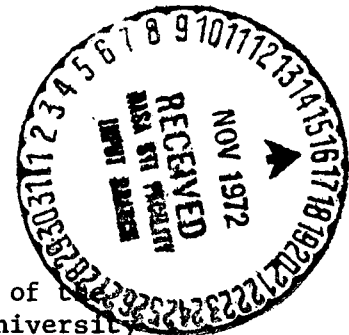


A NUMERICAL ANALYSIS OF THE TRANSIENT  
RESPONSE OF AN ABLATION SYSTEM  
INCLUDING EFFECTS OF THERMAL  
NON-EQUILIBRIUM, MASS TRANSFER  
AND CHEMICAL KINETICS

by Ronald Keith Clark



Thesis submitted to the Graduate Faculty of  
Virginia Polytechnic Institute and State University  
in Candidacy for the degree of

DOCTOR OF PHILOSOPHY

in

Mechanical Engineering

May 1972

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A NUMERICAL ANALYSIS OF THE TRANSIENT RESPONSE  
OF AN ABLATION SYSTEM INCLUDING EFFECTS OF  
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(ABSTRACT)

The differential equations governing the transient response of a one-dimensional ablative thermal protection system undergoing stagnation ablation are derived for the general case of thermal non-equilibrium between the pyrolysis gases and the char layer and kinetically controlled chemical reactions and mass transfer between the pyrolysis gases and the char layer. The boundary conditions are written for the particular case of stagnation heating with surface removal by oxidation or sublimation and pyrolysis of the uncharred layer occurring in a plane.

The governing equations and boundary conditions are solved numerically using the modified implicit method (Crank-Nicolson method). Numerical results are compared with exact solutions for a number of simplified cases. The comparison is favorable in each instance.

Numerical results are presented for a typical ablation system subjected to a square heat pulse. The effects of chemical reactions and mass transfer are pronounced.

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## LIST OF SYMBOLS

$A$	specific reaction rate constant for chemical reaction (various units) or radiant energy absorption of char layer ( $\text{W/m}^3$ )
$A'$	radiant energy absorption of pyrolysis gases ( $\text{W/m}^3$ ) or specific reaction rate constant for pyrolysis of uncharred material ( $\text{kg/m}^2\text{-sec}$ )
$A_i$	chemical species $i$
$[A_i]$	mole density of chemical species $i$ ( $\text{mole/m}^3$ )
$A_s$	specific surface area (area per unit volume) of char layer ( $1/\text{m}$ ) or specific reaction rate constant for surface removal by oxidation (various units)
$B$	activation energy for chemical reaction ( $^\circ\text{K}$ )
$B'$	activation energy for pyrolysis of uncharred layer ( $^\circ\text{K}$ )
$B_s$	activation energy for surface removal by oxidation ( $^\circ\text{K}$ )
$C$	mass fraction of oxygen in boundary layer
$\bar{C}$	normalized mass fraction of oxygen in boundary layer
$C_p$	heat capacity of pyrolysis gases at constant pressure ( $\text{J/mole-}^\circ\text{K}$ )
$\hat{C}_p$	heat capacity of pyrolysis gases at constant pressure, per unit mass ( $\text{J/kg-}^\circ\text{K}$ )
$\hat{C}_{p_{\text{HS}}}$	heat capacity per unit mass of heat sink at interface of uncharred material and insulation layer ( $\text{J/kg-}^\circ\text{K}$ )
$\hat{C}_{p_{\text{HSP}}}$	heat capacity per unit mass of heat sink at back of insulation layer ( $\text{J/kg-}^\circ\text{K}$ )
$C_{p_i}$	heat capacity of chemical species $i$ at constant pressure ( $\text{J/mole-}^\circ\text{K}$ )
$C_{p_s}$	heat capacity of solid at constant pressure ( $\text{J/mole-}^\circ\text{K}$ )

x

$\hat{C}_{p_s}$	heat capacity of solid at constant pressure, per unit mass (J/kg-°K)
$C_s$	solid carbon
D	chemical diffusivity of boundary layer (m <sup>2</sup> )
$\epsilon$	radiant energy emission of char layer (W/m <sup>3</sup> )
$\epsilon'$	radiant energy emission of pyrolysis gases (W/m <sup>3</sup> )
$\epsilon_1, \epsilon_2, \epsilon_3$	coefficients in linearized differential equation for char layer porosity
G	free energy of pyrolysis gases (J/mole)
$\vec{g}$	resultant external force acting on pyrolysis gases (N/kg)
$\vec{g}_i$	external force acting on chemical species i (N/kg)
H	enthalpy of pyrolysis gases (J/mole)
$\bar{H}$	normalized enthalpy of boundary layer fluid
$\hat{H}$	enthalpy of pyrolysis gases, per unit mass (J/kg)
$H_A$	volumetric convective heat transfer coefficient (W/m <sup>3</sup> -°K)
$H_c$	heat of sublimation of char layer (J/kg)
$\hat{H}_e$	enthalpy of boundary layer fluid at edge of boundary layer, per unit mass (J/kg)
$H_i$	enthalpy of chemical species i (J/mole)
$\hat{H}_i$	enthalpy of chemical species i, per unit mass (J/kg)
$H_s$	enthalpy of char layer (J/mole)
$\hat{H}_s$	enthalpy of char layer, per unit mass (J/kg)
$\hat{H}_{s_0}$	heat of formation of char layer at 0 °K, per unit mass (J/kg)
$H(T)_{O_2}$	enthalpy of O <sub>2</sub> at temperature T (J/mole)

$\hat{H}(T)_s$	enthalpy of solid at temperature T, per unit mass (J/kg)
$H(T_s)_{CO}$	enthalpy of CO at temperature $T_s$ (J/mole)
$H(T_s)_{C_s}$	enthalpy of solid carbon at temperature $T_s$ (J/mole)
I	number of finite difference stations in char layer
J	number of finite difference stations in uncharred layer
$J_i$	molar flux of chemical species i relative to mass average velocity (moles/m <sup>2</sup> -sec)
$j_i$	mass flux of chemical species i relative to mass average velocity (kg/m <sup>2</sup> -sec)
K	permeability of char layer (m <sup>2</sup> ) or number of finite difference stations in insulation layer
$K_h$	constant in equation for $H_A$ (Eq. 2-1) (1/m)
k	thermal conductivity of boundary layer fluid (W/m-°K) or specific reaction rate (various units)
$k_f$	forward reaction rate of chemical reaction (various units)
$k_r$	reverse reaction rate of chemical reaction (various units)
$k_s$	thermal conductivity of solid (W/m-°K)
$l$	thickness of char layer (m)
$l'$	thickness of uncharred layer (m)
$l''$	thickness of insulation layer (m)
$l_{HS}$	thickness of heat sink between uncharred layer and insulation layer (m)
$l_{HSP}$	thickness of heat sink at back of insulation layer (m)
$l_o$	initial thickness of char layer (m)
$l'_o$	initial thickness of uncharred layer (m)
$\bar{M}$	average molecular weight of pyrolysis gases (kg/mole)

$\dot{m}$	mass flow rate of pyrolysis gases ( $\text{kg/m}^2\text{-sec}$ )
$M_i$	molecular weight of chemical species $i$ ( $\text{kg/mole}$ )
$M_{O_2}$	molecular weight of $O_2$ ( $\text{kg/mole}$ )
$M_s$	molecular weight of char layer ( $\text{kg/mole}$ )
$\dot{m}_g$	rate of pyrolysis of uncharred material ( $\text{kg/m}^2\text{-sec}$ )
$\dot{m}_i$	mass flow rate of chemical species $i$ ( $\text{kg/m}^2\text{-sec}$ )
$\dot{m}_{O_2}$	mass rate of diffusion of $O_2$ through the boundary layer to the char layer surface ( $\text{kg/m}^2\text{-sec}$ )
$\dot{m}_s$	mass rate of char removal ( $\text{kg/m}^2\text{-sec}$ )
$\dot{m}_T$	effective rate of mass injection into the boundary layer ( $\text{kg/m}^2\text{-sec}$ )
$n$	order of chemical reaction
$\vec{n}$	unit vector normal to the surface
$\vec{n}_i$	mass flux of chemical species $i$ relative to a fixed coordinate system ( $\text{kg/m}^2\text{-sec}$ )
$N_{Le}$	dimensionless parameter ( $k/\rho C_p D$ ), Lewis Number
$N_{Pr}$	dimensionless parameter ( $\mu C_p/k$ ), Prandtl Number
$N_{Sc}$	dimensionless parameter ( $\mu/\rho D$ ), Schmidt Number
$P$	Laplace transform of $T'$ defined by $\int_0^\infty e^{-st} T'(X;t) dt$ or pressure ( $\text{N/m}^2$ )
$P_1$	pyrolysis gas pressure at finite difference station 1 ( $\text{N/m}^2$ )
$P_e$	pressure at edge of boundary layer ( $\text{N/m}^2$ )
$P_{O_2}$	partial pressure of $O_2$ ( $\text{N/m}^2$ )
$P_{w,o}$	initial pressure at char layer surface ( $\text{N/m}^2$ )
$P_{w,s}$	stagnation wall pressure ( $\text{N/m}^2$ )
$\vec{q}$	rate of energy transfer in pyrolysis gases by conduction ( $\text{W/m}^2$ )

$q'''$	rate of energy generated in pyrolysis gases by sources (W/m <sup>3</sup> )
$q_{\text{Aero}}$	net aerodynamic heating rate to the surface (W/m <sup>2</sup> )
$q_B$	net heating rate to the back surface of the insulation layer (W/m <sup>2</sup> )
$q_C$	cold wall convective heating rate to the front surface (W/m <sup>2</sup> )
$q_{C,\text{net}}$	net convective heating rate to the front surface (W/m <sup>2</sup> )
$q_R$	radiant heating rate to the front surface (W/m <sup>2</sup> )
$\vec{q}_s$	rate of energy transfer in solid by conduction (W/m <sup>2</sup> )
$q_s'''$	rate of energy generated in solid by sources (W/m <sup>2</sup> )
$r(r)$	net rate of progress of $r^{\text{th}}$ chemical reaction (1/m <sup>3</sup> -sec)
Rad	radius of curvature of surface (m)
$r_h(r)$	net rate of progress of $r^{\text{th}}$ heterogenous chemical reaction (1/m <sup>3</sup> -sec)
$R_{h_i}$	molar rate of production of chemical species $i$ by heterogeneous chemical reactions (moles/m <sup>3</sup> -sec)
$R_{h_s}$	molar rate of production of solid by heterogeneous chemical reactions (moles/m <sup>3</sup> -sec)
$r_{h_s}$	mass rate of production of solid by heterogeneous chemical reactions (kg/m <sup>3</sup> -sec)
$R_i$	molar rate of production of chemical species $i$ by homogeneous chemical reactions (moles/m <sup>3</sup> -sec)
$R_s$	molar rate of production of solid by homogeneous chemical reactions (moles/m <sup>3</sup> -sec)
$r_s$	mass rate of production of solid by homogeneous chemical reactions (kg/m <sup>3</sup> -sec)
$R_{T_i}$	net molar rate of production of chemical species $i$ (moles/m <sup>3</sup> -sec)

$r_{T_i}$	net mass rate of production of chemical species $i$ (kg/m <sup>3</sup> -sec)
$R_u$	universal gas constant (J/mole-°K)
$S$	surface area (m <sup>2</sup> ) or entropy of pyrolysis gases (J/mole-°K)
$s$	exponent on $T$ in chemical reaction rate equation (Eq. 2-67)
$\hat{S}$	entropy of pyrolysis gases per unit mass, (J/kg-K)
$\hat{S}_i$	entropy of chemical species $i$ per unit mass, (J/kg-K)
$S(T_{s_1} - \bar{T}_1)$	step function defined for use in Eq. 3-41
$T$	pyrolysis gas temperature (°K)
$t$	time (seconds)
$T'$	dimensionless temperature defined by Eq. 7-7
$\bar{T}_I$	maximum temperature of pyrolysis zone used when limiting temperature at that station (°K)
$T_o$	initial temperature of pyrolysis gases (°K) or reservoir temperature (°K)
$T_s$	solid temperature (°K)
$\bar{T}_1$	maximum char surface temperature used when limiting temperature at that station (°K)
$u$	component of velocity vector (m/sec)
$\hat{U}$	internal energy per unit mass of pyrolysis gases (J/kg)
$V$	volume (m <sup>3</sup> )
$\hat{V}$	volume of pyrolysis gases per unit mass (m <sup>3</sup> /kg)
$v$	component of velocity vector (m/sec) or velocity of pyrolysis gases in char layer (m/sec)
$V_c$	velocity of finite difference station in moving coordinate system (m/sec)



$v_o$	superficial velocity of pyrolysis gases in char layer (m/sec)
$v$	flow field velocity external of the boundary layer (m/sec)
$x$	dimensionless moving coordinate attached to the char layer surface
$x'$	dimensionless moving coordinate attached to the pyrolysis zone
$x''$	dimensionless coordinate attached to the uncharred layer-insulation layer interface
$x_d$	moving coordinate attached to the char layer surface (m)
$x'_d$	moving coordinate attached to the pyrolysis zone (m)
$x''_d$	coordinate attached to the uncharred layer-insulation layer interface (m)
$x_i$	mole fraction of chemical species $i$
$x_{O_2}$	mole fraction of $O_2$
$y$	fixed coordinate (m)
$z$	fixed coordinate (m)

Greek letters:

$\alpha$	absorptivity of front surface
$\alpha_c$	weighting factor for char material injected into boundary layer
$\alpha_p$	weighting factor for pyrolysis gases injected into boundary layer
$\alpha_1, \alpha_2, \alpha_3, \alpha_4$	coefficients in linearized differential equation for solid temperature
$\beta$	trigger for selecting blocking approximation; $\beta = 0$ for 2nd order approximation, $\beta = 1$ for linear approximation

$\beta_1, \beta_2, \beta_3$	coefficients in linearized differential equation for pyrolysis gas temperature
$\gamma_1, \gamma_2, \gamma_3, \gamma_4$	coefficients in linearized differential equation for pyrolysis gas pressure
$\bar{\delta}$	unit tensor
$\Delta_{1_i}, \Delta_{2_i}, \Delta_{3_i}$	coefficients in linearized chemical species conservation equation
$\Delta H$	heat of reaction for heterogeneous chemical reaction
$\Delta H_c$	heat of combustion of char (J/mole)
$\Delta H_p$	heat of pyrolysis of uncharred material (J/kg)
$\Delta t$	increment in time (sec)
$\Delta T_{\text{surface}}$	change in temperature of char layer surface ( $^{\circ}\text{K}$ )
$\Delta x$	dimensionless distance between finite difference stations
$\Delta \rho$	difference in density of uncharred material and char layer at the pyrolysis zone ( $\text{kg/m}^3$ )
$\epsilon_s$	emissivity of char surface
$\epsilon_s''$	emissivity of back surface
$\eta$	char layer porosity
$\eta_I$	char layer porosity at pyrolysis zone
$\eta_o$	initial char layer porosity
$\bar{\eta}$	blocking coefficient used with linear ablation theory
$\theta_j$	fraction of surface sites occupied by molecules of chemical species $j$
$\theta_o$	fraction of surface sites which are void
$\lambda$	ratio of char layer mass removed to mass of oxygen diffusing to the surface
$\mu$	viscosity of pyrolysis gases or boundary layer fluid ( $\text{N} - \text{sec/m}^2$ )

$\hat{\mu}_i$	chemical potential of chemical species $i$ (J/kg)
$v'_i$	coefficient of chemical species $i$ appearing as a reactant in a stoichiometric representation of a chemical reaction (moles)
$v''_i$	coefficient of chemical species $i$ appearing as a product in a stoichiometric representation of a chemical reaction (moles)
$\rho$	density of pyrolysis gases or boundary layer fluid (kg/m <sup>3</sup> )
$\bar{\rho}$	normalized density of boundary layer fluid
$\rho_{HS}$	density of heat sink at interface of uncharred layer and insulation layer (kg/m <sup>3</sup> )
$\rho_{HSP}$	density of heat sink at back of insulation layer (kg/m <sup>3</sup> )
$\rho_i$	density of chemical species $i$ (kg/m <sup>3</sup> )
$\rho_s$	density of solid (kg/m <sup>3</sup> )
$\rho_{s_0}$	density of char layer at the front surface (kg/m <sup>3</sup> )
$\rho_\infty$	flow field density external to the boundary layer (kg/m <sup>3</sup> )
$\sigma$	Stefan-Boltzmann constant (W/m <sup>2</sup> -sec-°K <sup>4</sup> )
$\bar{\tau}$	viscous stress tensor (N/m <sup>2</sup> )
$\tau_{xx}$	xx-element of the viscous stress tensor in moving coordinate system (N/m <sup>2</sup> )
$\tau_{yy}$	yy-element of the viscous stress tensor in fixed coordinate system (N/m <sup>2</sup> )

Overlines

-	normalized or averaged
^	per unit mass
→	vector
-	tensor

Superscripts

'	uncharred layer
"	insulation layer
P	at start of time step
$P+\Delta t$	at end of time step
$P+\Delta t/2$	at middle of time step
r	chemical reaction r

Subscripts

CO	carbon monoxide
$C_s$	solid carbon
e	free stream
f	forward direction
h	heterogeneous chemical reaction
hom	homogeneous chemical reaction
I	pyrolysis zone
i	chemical species i
I+J	interface of uncharred layer and insulation layer
I+J+K	back surface of insulation layer
N	station N
New	moving coordinate system
o	initial value
Old	initial fixed coordinate system
$O_2$	oxygen
r	reverse direction

s	solid or stagnation point
w	wall
l	char layer surface

## CHAPTER I

### INTRODUCTION

Space vehicles reentering the earth's atmosphere or entering other planetary environments are subjected to severe aerodynamic heating. Several methods of protecting the interior of the spacecraft have been proposed. Conditions resulting in high aerodynamic heating rates require use of ablation materials for thermal protection. The charring ablator thermal protection material (see schematic diagram, Fig. 1) has been found most effective as a thermal shielding material for a wide range of heating conditions. In Ref. 1 Swann discusses weights and efficiencies of various thermal protection systems for a range of heating conditions.

The favorable performance of the charring ablator is largely attributable to the tough char layer which forms on the surface of the material as it is heated. This char layer is capable of withstanding very high temperatures, and during reentry a significant amount of the total heat input at the surface is radiated to the environment by the high temperature char surface. Gases generated in the pyrolysis zone of the charring ablator percolate through the high temperature porous char layer to the surface. As these pyrolysis gases flow through the char layer, they absorb energy by increasing in temperature and undergoing chemical reactions.

The performance of ablative thermal protection systems has been the subject of extensive research over the past decade. Refs. 2, 3,

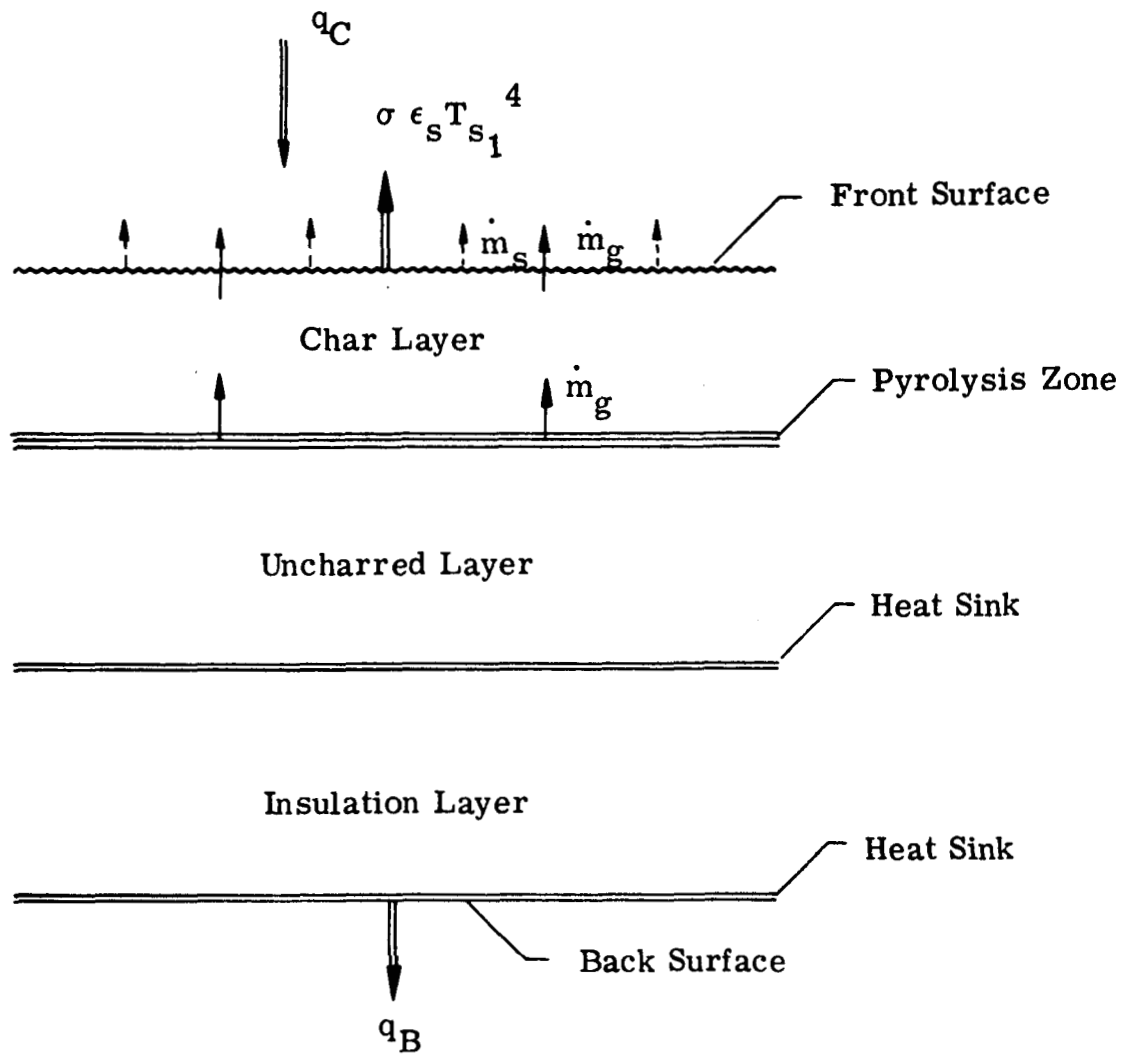


Figure 1.- Schematic diagram of charring ablator.

and 4 by Chapman, Dow and Tompkins , and Chapman and Dow are typical of the many reports presenting results of experimental evaluation of the ablative performance of thermal protection materials. The experimental programs whose results are reported in Refs. 2, 3 and 4 involved testing candidate thermal protection materials in arc-heated tunnels to compare their performance as thermal protection systems for reentry applications.

Many analytical reports have been devoted to developing theories of ablation. In Refs. 5, 6 and 7 Roberts considers the effects of mass transfer processes near the stagnation point on heat transfer to two-dimensional or axisymmetric bodies. Ref. 5 presents a simplified analysis of mass transfer cooling near the stagnation point for two dimensional or axisymmetric bodies, showing the reduction in heat transfer in terms of the properties of the cooling fluid. Ref. 6 presents a simplified analysis of the shielding mechanism which reduces the stagnation point heat transfer when ablation takes place at the surface. Ref. 7 presents a theoretical study of the shielding mechanism whereby the rates of heat transfer are reduced near the stagnation point of two-dimensional and three dimensional bodies when melting and vaporization occur simultaneously.

A large body of literature exists which describes the experimental and analytical effort directed toward studying the performance of ablative thermal protection systems including the interaction of the ablator with the boundary layer. In Ref. 8 Scala and Gilbert present



a theoretical analysis of the overall response of a char-forming plastic during hypersonic flight. The rate of pyrolysis of the plastic is calculated by means of a chemical kinetic equation. A mathematical description of the gas flow through the char is included. Hypersonic boundary layer mass transfer effects are also considered in the overall energy balance. Results are presented for the forward stagnation line of an unyawed cylinder in hypersonic flow undergoing quasi-steady ablation.

An analysis of the effects of environmental conditions on the performance of charring ablators is presented in Ref. 9 by Swann, Dow and Tompkins. Equations relating different environments which produce the same material response are derived for the case of surface removal by oxidation. The effects of environmental parameters on the thermal performance of ablators are examined.

In Ref. 10 Swann presents an analysis of the performance of char-forming ablators. It includes a derivation of the equations governing the response of charring ablators subject to char removal by diffusion controlled oxidation. Results are presented for the case of a constant enthalpy level and the effects of various material properties and environmental parameters are discussed.

A study of the effects of oxidation on the performance of charring ablators is presented in Ref. 11 by Dow and Swann. Char-forming ablation specimens were exposed to high energy gas streams of nitrogen and different oxygen concentrations. Surface removal data from these

tests were correlated in terms of a diffusion limited oxidation mechanism. An energy balance calculated for specimens exposed to 11.5 percent oxygen concentration showed that the heat input from combustion is a significant part of the total heat input.

Further attempts at defining the effects of environment and material properties on the performance of ablators are discussed by Clark in Ref. 12 and Swann, Brewer and Clark in Ref. 13.

Because of the many complex factors involved, the usefulness of developing computer simulation programs as a practical tool for solving ablation problems was obvious early in the previous decade. Early analyses of ablative thermal protection systems neglected or greatly simplified the complex processes and rate controlling mechanisms that occur in charring ablation systems. Ref. 14 by Swann and Pittman represents an early numerical treatment of an ablative thermal protection system. It presents a derivation in finite difference form of the energy transfer equations for a charring ablator system in which thermal equilibrium exists between the char layer and the pyrolysis gases. Removal of material at the surface by chemical and/or mechanical processes is achieved by modelling any of the following mechanisms:

- 1) ablation at a given temperature
- 2) material erosion as a given function of time
- 3) material erosion such that the char thickness is a given function of time.

Pyrolysis of the uncharred material occurs at a single given temperature, so that a well-defined interface exists between the char layer

and the uncharred layer. Reduction of aerodynamic heating at the surface resulting from injection of pyrolysis gases into the boundary layer is accounted for by using a second-degree approximation to the boundary layer solutions for air-to-air injection. The effect of chemical reactions involving the pyrolysis gases as they flow through the char layer is included by using an effective specific heat for the pyrolysis gases which is adjusted to account for endothermic and exothermic chemical processes. Ref. 14 presents some typical results from computer calculations and some comparisons with experimental results.

In Ref. 15 Kratsch, Hearne and McChesney present a sound effort at developing and experimentally verifying a theoretical model of a charring ablation thermal protection system. They present the coupled energy and mass transfer equations for a two-component resin-fabric composite with a complete description of the chemical processes involved. However, it invokes the assumption of thermal equilibrium between the char layer and pyrolysis gases. It also assumes steady state conditions exist. Experimental and computed results are presented for comparison.

Ref. 16 by Swann, Pittman and Smith presents what is perhaps the most widely employed numerical ablation analysis. Basically it represents a greatly improved version of the earlier analysis by Swann and Pittman (Ref. 14). The improvements include the following: (1) treatment of surface removal by chemical oxidation with consideration of rate controlled and diffusion controlled regimes; (2) pyrolysis

of the uncharred layer as an exponential function of temperature, and (3) transformation of governing equations to a moving coordinate system to accommodate changes in location of the surfaces of the ablator. However, their analysis also invokes the assumption of thermal equilibrium between the char layer and pyrolysis gases. Ref. 16 presents a comparison of computed results with exact solutions for simplified cases. The agreement between the numerical and exact solutions is good.

More recently strong interest has been directed toward the chemical processes occurring within the char layer of an ablation system. The experimental work by Clark which is reported in Refs. 17 and 18 demonstrates the intensity of these processes. This work also shows that the pyrolysis gases and char layer are not always in thermal equilibrium. Ref. 19 by Brewer, Stroud and Clark shows a thirty percent variation in thermal protection requirements for a typical reentry vehicle depending on whether the pyrolysis gases in the char are in chemical equilibrium or frozen as they flow from the pyrolysis zone to the surface.

This report presents an analysis of the transient response of a one-dimensional ablative thermal protection system undergoing stagnation ablation. The differential equations governing heat and mass transfer are derived out for both the char layer and the pyrolysis gases flowing through the char layer. These equations are coupled through a convective heat transfer term which represents energy transferred from the char layer to the pyrolysis gases. The

differential equation governing the pressure distribution in the char layer is formulated. Chemical rate equations describing the chemical reactions occurring in the char layer are formulated.

The boundary conditions are written for the particular case of stagnation heating with surface removal by oxidation and/or sublimation, and temperature dependent pyrolysis of the uncharred material occurring in a plane.

The governing equations and boundary conditions are solved numerically using a digital computer. Numerical solutions are obtained for a number of simple problems where exact solutions are available to test the integrity of various parts of the total program. Results are presented for a body subjected to stagnation heating with surface removal by oxidation and finite-rate chemistry occurring in the char layer to illustrate the form of results obtained using this tool. A discussion of the use of this program in design of thermal protection systems is included.

## CHAPTER II

### GOVERNING EQUATIONS

A charring ablator system can be described by three distinct layers as shown in Fig. 1. These layers are the char layer and the uncharred material, which make up the ablator, and the heat sink and substrate insulation which are behind the ablator. The char layer is exposed to aerodynamic and/or radiant heating at the front surface. The surface of the char layer may also interact with the external boundary layer resulting in erosion of the char layer by chemical reactions and/or mechanical means. The region separating the char layer and the uncharred material is labeled the pyrolysis zone and is assumed to be a plane. The uncharred material undergoes pyrolysis at this interface at a rate given by an empirical Arrhenius type relation producing gaseous pyrolysis products and a porous char layer. The gaseous products absorb energy and undergo chemical reactions as they flow through the porous char layer to the front surface where they are injected into the boundary layer. From this discussion it is seen to be necessary to consider the three layers separately in deriving the differential equations which govern the behavior of an ablative system.

The char layer consists of two phases - the porous solid residue or char and the gaseous pyrolysis products, or pyrolysis gases, flowing through the porous residue. The porous residue experiences heat conduction and mass and heat transfer from interaction with the flow of

pyrolysis products. The pyrolysis products flowing through the porous residue undergo chemical reactions in addition to interacting with the solid. The uncharred layer and the substrate insulation experience heat conduction only.

#### Char Layer Equations

The char layer requires two differential equations for conservation of energy - one for the char and one for the pyrolysis gases. Mass transfer processes affecting the char must be considered to obtain an equation for variation of the char porosity. The pyrolysis gases also require differential equations for conservation of chemical species, total mass and momentum, and chemical reaction rate equations.

Char temperature differential equation.-The energy conservation equation for the char is obtained by considering a control volume  $V$  within the char layer. The char occupies a fraction of this volume equal to  $(1 - \eta)$  where  $\eta$  is the char layer porosity. The energy conservation equation applied to the solid phase of the char layer states that the rate of change of energy contained in the solid phase of the char within the control volume  $V$  equals the sum of the net ratio of energy transfer into the solid phase by conduction heat transfer, convection to the pyrolysis gases, mass transfer from the pyrolysis gases to the solid resulting from homogeneous chemical reactions and heterogeneous chemical reactions (reactions occurring on the solid surface), heats of reaction given up by the solid in heterogeneous chemical reactions involving the pyrolysis gases and

the solid, radiation of energy to the solid and energy produced within the solid by any internal source.

The total energy contained in the solid phase of the char within a unit volume of the char layer is equal to the product of the theoretical solid density, enthalpy and solid phase volume fraction which is  $(1 - \eta)$ . The terms of the char energy equation may be written as follows:

Non-stationary volume term

$$\int_V \frac{\partial}{\partial t} [(1 - \eta) \rho_s \hat{H}_s] dV$$

Conduction heat transfer term

$$- \int_S \vec{q}_s \cdot \vec{n} dS$$

Convection to the pyrolysis gases

$$- \int_V H_A (T_s - T) dV$$

where the volumetric heat transfer coefficient for convective energy transfer from the char to the pyrolysis gases is given by Bland in Ref. 20 as

$$H_A = \frac{K_h v}{N_{Pr}} \sum_i \frac{\rho_i C_{pi}}{M_i} \quad (2-1)$$



Mass transfer from the pyrolysis gases to the solid resulting from homogeneous chemical reactions

$$\int_V \eta r_s \hat{H}(T)_s dV$$

Mass transfer from the pyrolysis gases to the solid resulting from heterogeneous chemical reactions

$$\int_V \eta r_{hs} \hat{H}_s dV$$

Heats of reaction given up by the solid in heterogeneous chemical reactions

$$- \int_V \eta \sum_r r_h^{(r)} \Delta H^{(r)} dV$$

Radiation of energy to the solid

$$\int_V (1 - \eta)(A - \epsilon) dV$$

Energy produced within the solid by any internal source

$$\int_V (1 - \eta) q_s''' dV$$

Combining these terms in equation form gives

$$\begin{aligned}
\int_V \frac{\partial}{\partial t} [(1 - \eta) \rho_s \hat{H}_s] dV = & - \int_S \vec{q}_s \cdot \vec{n} dS - \int_V H_A (T_s - T) dV \\
& + \int_V \eta r_s \hat{H}(T_s) dV + \int_V \eta r_{hs} \hat{H}_s dV - \int_V \eta \sum_r r_h^{(r)} \Delta H^{(r)} dV \\
& + \int_V (1 - \eta)(A - \epsilon) dV + \int_V (1 - \eta) q_s''' dV
\end{aligned} \tag{2-2}$$

which is a statement of conservation of thermal and chemical energy for the portion of a control volume in the char layer occupied by solid. The energy term associated with stresses has not been included since that term is negligible with respect to other terms. The use of enthalpy in this equation is consistent with its nearly universal usage as a measure of the energy content of solids; however, implicit with its use is the assumption that enthalpy and internal energy are equal. This assumption is valid for incompressible solids.

The term associated with the heats of reaction for heterogeneous chemical reactions is obtained by assuming that the heat of reaction for each reaction is supplied by the char. As an example, consider the  $r^{\text{th}}$  heterogeneous chemical reaction which is the oxidation of solid carbon to form carbon monoxide. The stoichiometric equation representing this reaction is



and the heat supplied to the reaction is just the difference in enthalpy of the products and the reactants, or in equation form

$$\Delta H^{(r)} = 2 H(T_s)C_O - H(T)O_2 - H(T_s)C_s \quad (2-4)$$

Applying Gauss's Theorem to the surface integral to obtain a volume integral results in the following equation

$$\int_V \left\{ \frac{\partial}{\partial t} [(1 - \eta) \rho_s \hat{H}_s] + \vec{\nabla} \cdot \vec{q}_s + H_A (T_s - T) - \eta r_s \hat{H}(T)_s - \eta r_{hs} \hat{H}_s \right. \\ \left. + \eta \sum_r r_h^{(r)} \Delta H^{(r)} - (1 - \eta)(A - \epsilon) - (1 - \eta) q''' \right\} dV = 0. \quad (2-5)$$

This equation is true for any volume  $V$ ; therefore, the integral can vanish only if the integrand vanishes everywhere. Thus, the differential form of the char energy equation is

$$\frac{\partial}{\partial t} [(1 - \eta) \rho_s \hat{H}_s] + \vec{\nabla} \cdot \vec{q}_s + H_A (T_s - T) - \eta r_s \hat{H}(T)_s - \eta r_{hs} \hat{H}_s \\ + \eta \sum_r r_h^{(r)} \Delta H^{(r)} - (1 - \eta)(A - \epsilon) - (1 - \eta) q''' = 0. \quad (2-6)$$

The non-stationary term is expanded to obtain

$$\frac{\partial}{\partial t} [(1 - \eta) \rho_s \hat{H}_s] = (1 - \eta) \rho_s \frac{\partial \hat{H}_s}{\partial t} + (1 - \eta) \hat{H}_s \frac{\partial \rho_s}{\partial t} - \rho_s \hat{H}_s \frac{\partial \eta}{\partial t}. \quad (2-7)$$

But the theoretical density of the char is constant; therefore,

$$\frac{\partial}{\partial t} [(1 - \eta) \rho_s \hat{H}_s] = (1 - \eta) \rho_s \frac{\partial \hat{H}_s}{\partial t} - \rho_s \hat{H}_s \frac{\partial \eta}{\partial t}. \quad (2-8)$$

The char layer energy equation now takes the form

$$(1 - \eta) \rho_s \frac{\partial \hat{H}_s}{\partial t} = - \vec{\nabla} \cdot \vec{q}_s - H_A (T_s - T) + \eta r_s \hat{H}(T)_s + \eta r_{hs} \hat{H}_s - \eta \sum_r r_r^{(r)} \Delta H^{(4)} + (1 - \eta)(A - \epsilon) + (1 - \eta) q_s''' + \rho_s \hat{H}_s \frac{\partial \eta}{\partial t} . \quad (2-9)$$

It is more convenient to work with temperature than enthalpy. The char enthalpy may be written as

$$\hat{H}_s = \int_0^{T_s} \hat{C}_{p_s} dT_s + \hat{H}_{s_o} . \quad (2-10)$$

The time rate of change of char enthalpy is obtained by differentiating Eq. 2-10,

$$\frac{\partial \hat{H}_s}{\partial t} = \frac{\partial}{\partial t} \int_0^{T_s} \hat{C}_{p_s} dT_s + \frac{\partial}{\partial t} \hat{H}_{s_o} . \quad (2-11)$$

The derivative of the integral appearing here is obtained by applying the Leibnitz Rule for differentiation under the integral sign as in Hildebrand (Ref. 21). Thus Eq. 2-11 becomes

$$\frac{\partial \hat{H}_s}{\partial t} = \int_0^{T_s} \frac{\partial}{\partial t} \hat{C}_{p_s} dT_s + \hat{C}_{p_s} \frac{\partial T_s}{\partial t} + \frac{\partial}{\partial t} \hat{H}_{s_o} , \quad (2-12)$$

but  $\hat{C}_{ps}$  is not a function of time and  $\hat{H}_{s_0}$  is constant so

$$\frac{\partial \hat{H}_s}{\partial t} = \hat{C}_{ps} \frac{\partial T_s}{\partial t} . \quad (2-13)$$

Combining Eq. 2-13 and Fourier's conduction equation,

$$\vec{q}_s = -k_s \vec{\nabla} T_s , \quad (2-14)$$

with Eq. 2-9 gives the differential equation for conservation of energy in the char layer as

$$\begin{aligned} (1 - \eta) \rho_s \hat{C}_{ps} \frac{\partial T_s}{\partial t} = \vec{\nabla} \cdot (k_s \vec{\nabla} T_s) - H_A (T_s - T) + \eta r_s \hat{H}(T)_s \\ + \eta r_{hs} \hat{H}_s - \eta \sum_r r_h^{(r)} \Delta H^{(r)} + (1 - \eta)(A - \epsilon) \\ + (1 - \eta) q_s''' + \rho_s \hat{H}_s \frac{\partial \eta}{\partial t} . \end{aligned} \quad (2-15)$$

The specific quantities  $\hat{C}_{ps}$ ,  $\hat{H}_s(T)$ ,  $\Delta H_j$  and  $\hat{H}_s$  and the chemical production terms  $r_s$  and  $r_{hs}$  may be expressed in terms of the respective mole quantities and Eq. 2-15 becomes

$$\begin{aligned} (1 - \eta) \frac{\rho_s C_{ps}}{M_s} \frac{\partial T_s}{\partial t} = \vec{\nabla} \cdot (k_s \vec{\nabla} T_s) - H_A (T_s - T) + \eta R_s H(T)_s \\ + \eta R_{hs} H_s - \eta \sum_r r_h^{(r)} \Delta H^{(r)} + (1 - \eta)(A - \epsilon) \\ + (1 - \eta) q_s''' + \frac{\rho_s H_s}{M_s} \frac{\partial \eta}{\partial t} . \end{aligned} \quad (2-16)$$

Char porosity differential equation.— The porosity differential equation results from consideration of mass transfer between the char and the pyrolysis gases. Mass transfer between these two phases results from two sources. One source is the solid material formed by homogeneous chemical reactions in the pyrolysis gases. This solid material is deposited from the gas phase to the solid phase. The other source is the solid material formed or consumed by heterogeneous chemical reactions which occur at the char-gas interface.

The rate of formation of solid material by homogeneous chemical reactions in the pyrolysis gases is determined from the appropriate chemical reaction rate equations to be  $R_s$  (moles solid per unit volume of gas per unit time). The product of the char porosity (void fraction of the char layer), the molecular weight of the solid, and the rate of formation of solid gives the rate of material deposited in mass units per unit volume of char layer. Or, in equation form

$$\text{Mass Rate of Deposition} = \eta M_s R_s . \quad (2-17)$$

This deposit occupies a volume equal to  $\frac{1}{\rho_s}$  volume units per unit mass and this volume represents a decrease in the porosity of the char layer. Thus the time rate of change of char porosity due to homogeneous chemical reactions is

$$\left( \frac{\partial \eta}{\partial t} \right)_{\text{hom}} = - \eta \frac{M_s R_s}{\rho_s} . \quad (2-18)$$

Similarly, the rate of formation of solid by heterogeneous chemical reactions,  $R_{hs}$ , is determined from the appropriate chemical reaction rate equations. Thus the time rate of change of char porosity due to heterogeneous chemical reactions is

$$\left(\frac{\partial \eta}{\partial t}\right)_h = - \eta \frac{M_s}{\rho_s} R_{hs} . \quad (2-19)$$

Summing Eqs. 2-18 and 2-19 gives the time rate of change of char layer porosity as

$$\frac{\partial \eta}{\partial t} = - \frac{\eta M_s}{\rho_s} (R_{hs} + R_s) . \quad (2-20)$$

Pyrolysis gas energy differential equation.— The energy conservation equation applied to the fluid phase of the char layer states that the time rate of change of internal and kinetic energy contained in the pyrolysis gases within the control volume  $V$  equals the sum of the net rates of convection of internal and kinetic energy transferred into the pyrolysis gases due to the mass average velocity, conduction of energy in the pyrolysis gases, radiation of energy to the pyrolysis gases, work done on the pyrolysis gases by external forces, work done on the pyrolysis gases by pressure forces, work done on the pyrolysis gases by viscous forces, energy transfer to the pyrolysis gases by convection from the char, energy loss by the pyrolysis gases due to mass transfer and energy gained by the pyrolysis gases due to

heterogeneous chemical reactions. The terms of the pyrolysis gas energy equation may be written as follows:

Non-stationary volume term

$$\int_V \frac{\partial}{\partial t} [\eta \rho (\hat{U} + \frac{1}{2} v^2)] dV$$

Convection by mass average velocity

$$-\int_S (\hat{U} + \frac{1}{2} v^2) \rho \vec{v}_o \cdot \vec{n} dS$$

where  $v$  is the velocity of the pyrolysis gases in the char layer and  $v_o$  is the superficial velocity (volume rate of flow through a unit cross-sectional area of the char plus pyrolysis gases).

Conduction term

$$-\int_S \vec{q} \cdot \vec{n} dS$$

Radiation term

$$\int_V \eta (A' - \epsilon') dV$$

Work by external forces

$$\int_V \eta \sum_i \vec{n}_i \cdot \vec{g}_i dV$$



where  $\vec{n}_i$  is a mass flux vector equal to the sum of the mass flux due to mass average velocity and the mass flux due to diffusion, or in equation form

$$\vec{n}_i = \rho_i \vec{v} + \vec{j}_i \quad (2-21)$$

Work by pressure forces

$$- \int_S P \vec{v}_o \cdot \vec{n} \, dS$$

Work by viscous forces

$$\int_S [\vec{\tau} \cdot \vec{v}_o] \cdot \vec{n} \, dS$$

Convection from the char

$$\int_V H_A (T_s - T) \, dV$$

Energy loss by mass transfer resulting from homogeneous chemical reactions

$$- \int_V \eta r_s \hat{H}(T)_s \, dV$$

Energy loss by mass transfer resulting from heterogeneous chemical reactions

$$- \int_V \eta \, r_{hs} \, \hat{H}_s \, dV$$

Energy gain resulting from heterogeneous chemical reactions

$$\int_V \eta \sum_r r_h^{(r)} \Delta H^{(r)} \, dV \dots$$

Combining these terms in equation form gives

$$\begin{aligned} & \int_V \frac{\partial}{\partial t} \left[ \eta \rho \left( \hat{U} + \frac{1}{2} v^2 \right) \right] dV = \\ & - \int_S \left( \hat{U} + \frac{1}{2} v^2 \right) \rho \vec{v}_o \cdot \vec{n} \, dS - \int_S \vec{q} \cdot \vec{n} \, dS \\ & + \int_V \eta (A' - \epsilon') dV + \int_V \eta \sum_i \vec{n}_i \cdot \vec{g}_i \, dV \\ & - \int_S P \vec{v}_o \cdot \vec{n} \, dS + \int_S [\vec{\tau} \cdot \vec{v}_o] \cdot \vec{n} \, dS \\ & + \int_V H_A (T_s - T) \, dV - \int_V \eta \, r_s \, \hat{H}(T)_s \, dV \\ & - \int_V \eta \, r_{hs} \, \hat{H}_s \, dV + \int_V \eta \sum_r r_h^{(r)} \Delta H^{(r)} \, dV . \end{aligned} \tag{2-22}$$

Applying Gauss' Theorem to convert the surface integrals to volume integrals gives

$$\begin{aligned}
& \int_V \left\{ \frac{\partial}{\partial t} \left[ \eta \rho \left( \hat{U} + \frac{1}{2} v^2 \right) \right] + \vec{\nabla} \cdot \left[ \left( \hat{U} + \frac{1}{2} v^2 \right) \rho \vec{v}_o \right] \right. \\
& + \vec{\nabla} \cdot \vec{q} - \eta (A' - \epsilon') - \eta \sum_i \vec{n}_i \cdot \vec{g}_i + \vec{\nabla} \cdot P \vec{v}_o \\
& - \vec{\nabla} \cdot [\vec{\tau} \cdot \vec{v}_o] - H_A(T_s - T) + \eta r_s \hat{H}(T)_s + \eta r_{hs} \hat{H}_s \\
& \left. - \eta \sum_r r_r^{(r)} \Delta H^{(r)} \right\} dV = 0 \quad . \quad (2-23)
\end{aligned}$$

This equation is true for any volume  $V$ ; therefore, the integral can vanish only if the integrand vanishes everywhere. Thus the differential form of the pyrolysis gas internal and kinetic energy equation is

$$\begin{aligned}
& \frac{\partial}{\partial t} \left[ \eta \rho \left( \hat{U} + \frac{1}{2} v^2 \right) \right] + \vec{\nabla} \cdot \left[ \left( \hat{U} + \frac{1}{2} v^2 \right) \rho \vec{v}_o \right] + \vec{\nabla} \cdot \vec{q} \\
& - \eta (A' - \epsilon) - \eta \sum_i \vec{n}_i \cdot \vec{g}_i + \vec{\nabla} \cdot P \vec{v}_o \\
& - \vec{\nabla} \cdot [\vec{\tau} \cdot \vec{v}_o] - H_A(T_s - T) + \eta r_s \hat{H}(T)_s + \eta r_{hs} \hat{H}_s \\
& - \eta \sum_r r_h^{(r)} \Delta H^{(r)} = 0 \quad , \quad (2-24)
\end{aligned}$$

This equation can be simplified by subtracting from it the equation of mechanical energy. The equation of mechanical energy for

a fluid flowing through porous media results from taking the scalar product of the fluid velocity with the equation of motion. The equation of motion for a fluid flowing through porous media states that the time rate of change of momentum contained in the pyrolysis gas within the control volume  $V$  equals the sum of the net rates of momentum increase resulting from momentum convection by mass average velocity, pressure force per unit volume of pyrolysis gases, viscous transfer per unit volume of pyrolysis gases and gravitational force per unit volume of pyrolysis gases. In equation form

$$\begin{aligned} \int_V \frac{\partial}{\partial t} (\eta \rho \vec{v}) dV = & - \int_S (\rho \vec{v}) \vec{v}_o \cdot \vec{n} dS - \int_S \eta P \vec{\sigma} \cdot \vec{n} dS \\ & + \int_S \eta \vec{\tau} \cdot \vec{n} dS + \int_V \eta \rho \vec{g} dV . \end{aligned} \quad (2-25)$$

Gauss's theorem may be applied to Eq. 2-25 to convert the surface integrals to volume integrals giving

$$\begin{aligned} \int_V \left\{ \frac{\partial}{\partial t} (\eta \rho \vec{v}) + \vec{\nabla} \cdot \rho \vec{v} \vec{v}_o + \vec{\nabla} \eta P \right. \\ \left. - \vec{\nabla} \cdot \eta \vec{\tau} - \eta \rho \vec{g} \right\} dV = 0 . \end{aligned} \quad (2-26)$$

This equation is true for any volume  $V$ ; therefore, the integral can vanish only if the quantity in brackets vanishes everywhere. Thus the

differential form of the equation of motion for flow through porous media is

$$\begin{aligned} \frac{\partial}{\partial t} (\eta \rho \vec{v}) + \vec{\nabla} \cdot \rho \vec{v} \vec{v}_o + \vec{\nabla} \eta P \\ - \vec{\nabla} \cdot \eta \vec{\tau} - \eta \rho \vec{g} = 0 \end{aligned} \quad (2-27)$$

Forming the scalar product of the pyrolysis gas velocity with Eq. 2-27 gives the equation of mechanical energy for the pyrolysis gases as

$$\begin{aligned} \frac{1}{2} \frac{\partial}{\partial t} (\eta \rho v^2) + \frac{1}{2} \eta v^2 \frac{\partial \rho}{\partial t} + \frac{1}{2} \rho v^2 \frac{\partial \eta}{\partial t} + \frac{1}{2} \vec{\nabla} \cdot \rho v^2 \vec{v}_o \\ + \frac{1}{2} v^2 \vec{v}_o \cdot \vec{\nabla} \rho + \frac{1}{2} \rho v^2 \vec{\nabla} \cdot \vec{v}_o + \vec{\nabla} \cdot P \vec{v}_o \\ - \eta P \vec{\nabla} \cdot \vec{v} - \vec{\nabla} \cdot [\vec{\tau} \cdot \vec{v}_o] + \eta \vec{\tau} : \vec{\nabla} \cdot \vec{v} \\ - \eta \rho v g = 0 \end{aligned} \quad (2-28)$$

Equation 2-28 is subtracted from Eq. 2-24 to obtain the thermal energy equation of the pyrolysis gases as

$$\begin{aligned}
& \eta \rho \frac{D\hat{U}}{Dt} + \rho(\hat{U} - \frac{1}{2} v^2) \frac{D\eta}{Dt} + \eta(\hat{U} - \frac{1}{2} v^2) \left( \frac{D\rho}{Dt} + \rho \vec{\nabla} \cdot \vec{v} \right) \\
& + \eta P \vec{\nabla} \cdot \vec{v} - \eta \vec{\tau} : \nabla \vec{v} - \eta \sum_i \vec{j}_i \cdot \vec{g}_i + \vec{\nabla} \cdot \vec{q} \\
& - \eta (A' - \epsilon') - H_A(T_s - T) + \eta r_s \hat{H}(T)_s + \eta r_{hs} \hat{H}_s \\
& - \eta \sum_r r_h^{(r)} \Delta H_j^{(r)} = 0 .
\end{aligned} \tag{2-29}$$

Equation 2-29 can be simplified somewhat by expressing the internal energy in terms of the enthalpy and the state variables pressure and density and by making use of the mass conservation equation. The internal energy-enthalpy relation

$$\hat{U} = \hat{H} - P/\rho \tag{2-30}$$

yields

$$\frac{D\hat{U}}{Dt} = \frac{D\hat{H}}{Dt} - \frac{1}{\rho} \frac{DP}{Dt} + \frac{P}{\rho^2} \frac{D\rho}{Dt} , \tag{2-31}$$

Chemical species continuity equation.— The chemical species continuity equation applied to the pyrolysis gases flowing through the char layer states that the time rate of change of mass of some species within the control volume  $V$  equals the sum of the net rate of mass of that chemical species transferred into the control volume

by the mass average velocity and mass diffusion and the net rate of formation of that chemical species by chemical processes. Writing this equation in integral form gives

$$\begin{aligned} \int_V \frac{\partial}{\partial t} (\eta \rho_i) dV = & - \int_S \rho_i \vec{v}_o \cdot \vec{n} dS \\ & + \int_V \eta r_{T_i} dV - \int_S \eta \vec{j}_i \cdot \vec{n} dS . \end{aligned} \quad (2-32)$$

Applying Gauss's Theorem to convert the surface integrals to volume integrals gives

$$\int_V \left[ \frac{\partial}{\partial t} (\eta \rho_i) + \vec{\nabla} \cdot (\rho_i \vec{v}_o) - \eta r_{T_i} + \vec{\nabla} \cdot \eta \vec{j}_i \right] dV = 0 \quad (2-33)$$

which yields the chemical species conservation equation

$$\frac{\partial}{\partial t} (\eta \rho_i) + \vec{\nabla} \cdot (\rho_i \vec{v}_o) + \vec{\nabla} \cdot \eta \vec{j}_i - \eta r_{T_i} = 0 . \quad (2-34)$$

Total mass conservation equation.— The total mass conservation equation is obtained by summing the chemical species conservation equation over all species. Thus

$$\frac{\partial}{\partial t} (\eta \rho) + \vec{\nabla} \cdot (\rho \vec{v}_o) - \eta \sum_i r_{T_i} = 0 . \quad (2-35)$$

Equations 2-29, 2-31 and 2-35 are combined to give the pyrolysis gas energy equation in terms of enthalpy as

$$\begin{aligned}
 \eta \rho \frac{D\hat{H}}{Dt} = & \eta \frac{DP}{Dt} + P \frac{D\eta}{Dt} - \eta \left( \hat{H} - \frac{1}{2} v^2 \right) \sum r_{T_i} \\
 & + \eta \bar{\tau} : \vec{\nabla} \vec{v} + \eta \sum_i \vec{j}_i \cdot \vec{g}_i - \vec{\nabla} \cdot \vec{q} + \eta (A' - \epsilon') \\
 & + H_A (T_s - T) - \eta r_s \hat{H}(T)_s - \eta r_{hs} \hat{H}_s \\
 & + \eta \sum_r r_h^{(r)} \Delta H^{(r)} .
 \end{aligned} \tag{2-36}$$

It is more convenient to work with the pyrolysis gas energy equation written in terms of  $\hat{C}_p$  rather than  $\hat{H}$ . The desired form of the pyrolysis gas energy equation is obtained by combining Eq. 2-36 with the Gibbs equation written in terms of  $\hat{H}$  and the First Law of Thermodynamics.

The Gibbs equation for a system in equilibrium as written by Hatsopoulos and Keenan (Ref. 22) is

$$d\hat{H} = T d\hat{S} + \hat{V} dP + \sum_i \hat{\mu}_i d(\rho_i/\rho) . \tag{2-37}$$

It will now be assumed that, although the pyrolysis gases are not in true equilibrium, there exists within small mass elements a state of local equilibrium for which a bulk gas temperature can be defined and for which the local entropy  $\hat{S}$  is a well-defined function of the



various parameters which are necessary to define the macroscopic state of the system completely. With this assumption Eq. 2-37 becomes valid for a mass element followed along its center of motion, thus

$$\frac{D\hat{H}}{Dt} = T \frac{D\hat{S}}{Dt} + \hat{V} \frac{DP}{Dt} + \sum_i \hat{\mu}_i \frac{D}{Dt} (\rho_i/\rho) . \quad (2-38)$$

Equation 2-38 can be made more useful by expressing entropy in terms of  $P$ ,  $\hat{V}$  and  $T$ . Assuming the system is composed of a mixture of thermally perfect gases the entropy may be expressed as a function of  $P$ ,  $T$ , and  $\frac{\rho_i}{\rho}$ , or

$$\hat{S} = \hat{S}(P, T, \rho_i/\rho) \quad (2-39)$$

which yields

$$\begin{aligned} d\hat{S} = & \left( \frac{\partial \hat{S}}{\partial P} \right)_{T, \rho_i/\rho} dP + \left( \frac{\partial \hat{S}}{\partial T} \right)_{P, \rho_i/\rho} dT \\ & + \sum_i \left( \frac{\partial \hat{S}}{\partial \rho_i/\rho} \right)_{P, T} d(\rho_i/\rho) . \end{aligned} \quad (2-40)$$

Writing Eq. 2-37 in terms of specific heat

$$d\hat{S} = \frac{\hat{C}_P}{T} dT - \frac{\hat{V}}{T} dP - \frac{1}{T} \sum_i \hat{\mu}_i d(\rho_i/\rho) . \quad (2-41)$$

Equating the coefficients for  $dT$  in Eqs. 2-40 and 2-41 gives

$$\left( \frac{\partial \hat{S}}{\partial T} \right)_{P, \rho_i / \rho} = \frac{\hat{C}_P}{T} . \quad (2-42)$$

The coefficient of  $dP$  in Eq. 2-40 is replaced by its equivalent from the Maxwell relation

$$\left( \frac{\partial \hat{S}}{\partial P} \right)_{T, \rho_i / \rho} = - \left( \frac{\partial \hat{V}}{\partial T} \right)_{P, \rho_i / \rho} . \quad (2-43)$$

Equations 2-40, 2-42 and 2-43 are combined to give a differential entropy expression in terms of  $P$ ,  $\hat{V}$  and  $T$ .

$$d\hat{S} = \frac{\hat{C}_P}{T} dT - \left( \frac{\partial \hat{V}}{\partial T} \right)_{P, \rho_i / \rho} dT + \sum_i \left( \frac{\partial \hat{S}}{\partial \rho_i / \rho} \right)_{P, T} d(\rho_i / \rho) . \quad (2-44)$$

This equation may be written for a mass element followed along its center of motion as

$$\frac{D\hat{S}}{Dt} = \frac{\hat{C}_P}{T} \frac{DT}{Dt} - \left( \frac{\partial \hat{V}}{\partial T} \right)_{P, \rho_i / \rho} \frac{DP}{Dt} + \sum_i \left( \frac{\partial \hat{S}}{\partial \rho_i / \rho} \right)_{P, T} \frac{D}{Dt} (\rho_i / \rho) . \quad (2-45)$$

Equation 2-45 may be combined with Eq. 2-38 to give

$$\begin{aligned} \frac{D\hat{H}}{Dt} &= \hat{C}_P \frac{DT}{Dt} + \hat{V} \frac{DP}{Dt} - T \left( \frac{\partial \hat{V}}{\partial T} \right)_{P, \rho_i / \rho} \frac{DP}{Dt} \\ &+ \sum_i [\hat{\mu}_i + T \left( \frac{\partial \hat{S}}{\partial \rho_i / \rho} \right)_{P, T}] \frac{D}{Dt} (\rho_i / \rho) . \end{aligned} \quad (2-46)$$

The summation term in this equation can be reduced by considering the relation between partial properties. The entropy of a system is written as

$$\hat{S} = \sum_i (\rho_i / \rho) \hat{S}_i . \quad (2-47)$$

From Eq. 2-47 we have that

$$d\hat{S} = \sum_i \frac{\rho_i}{\rho} d\hat{S}_i + \sum_i \hat{S}_i d\left(\frac{\rho_i}{\rho}\right) . \quad (2-48)$$

Since entropy of a pure substance may be expressed as a function of  $P$  and  $T$ , Eq. 2-48 written for a constant pressure and temperature process is

$$d\hat{S} = \sum_i \hat{S}_i d(\rho_i / \rho) . \quad (2-49)$$

Thus

$$\left( \frac{\partial \hat{S}}{\partial \rho_i / \rho} \right)_{P,T} = \hat{S}_i . \quad (2-50)$$

The partial specific Gibbs function is defined as

$$\hat{\mu}_i = \left( \frac{\partial G}{\partial M_i} \right)_{P,T} . \quad (2-51)$$

But

$$G = H - TS \quad (2-52)$$

or

$$G = \sum_i M_i (\hat{H}_i - T \hat{S}_i) . \quad (2-53)$$

Equation 2-53 is combined with Eq. 2-51 to give the partial specific Gibbs function as

$$\hat{\mu}_i = \hat{H}_i - T \hat{S}_i . \quad (2-54)$$

Equations 2-50 and 2-54 are combined with Eq. 2-46 to satisfy the First Law of Thermodynamics applied to an element of mass near equilibrium followed along its center of motion. In equation form

$$\begin{aligned} \frac{D\hat{H}}{Dt} = \hat{C}_p \frac{DT}{Dt} + \hat{V} \frac{DP}{Dt} - T \left( \frac{\partial \hat{V}}{\partial T} \right)_{P, \rho_i / \rho} \frac{DP}{Dt} \\ + \sum_i \hat{H}_i \frac{D}{Dt} (\rho_i / \rho) . \end{aligned} \quad (2-55)$$

Equation 2-55 is combined with Eq. 2-36 to give the pyrolysis gas energy equation in terms of  $\hat{C}_p$  as

$$\begin{aligned}
\eta \rho \hat{C}_p \frac{DT}{Dt} = & - \eta \left( \frac{\partial \ln \rho}{\partial \ln T} \right) P, \rho_i / \rho \frac{DP}{Dt} - \eta \rho \sum_i \hat{H}_i \frac{D}{Dt} (\rho_i / \rho) \\
& + P \frac{D\eta}{Dt} - \eta \left( \hat{H} - \frac{1}{2} v^2 \right) \sum_i r_{T_i} + \eta \bar{\tau} : \vec{\nabla} \vec{v} + \eta \sum_i \vec{j}_i \cdot \vec{g}_i \\
& - \vec{\nabla} \cdot \vec{q} + \eta (A' - \epsilon') + H_A (T_s - T) - \eta r_s \hat{H}(T)_s - \eta r_{hs} \hat{H}_s \\
& + \eta \sum_{r,h} r^{(r)}_{h} \Delta H^{(r)} .
\end{aligned} \tag{2-56}$$

The derivative of  $\frac{\rho_i}{\rho}$  can be expanded and combined with the chemical species and total mass continuity equations (Eqs. 2-34 and 2-35) to give

$$\frac{D}{Dt} (\rho_i / \rho) = \frac{1}{\rho} r_{T_i} - \frac{1}{\eta \rho} \vec{\nabla} \cdot \vec{j}_i - \frac{\rho_i}{\rho^2} \sum_i r_{T_i} . \tag{2-57}$$

Equation 2-57 is combined with Eq. 2-56 and the specific quantities  $\hat{C}_p$ ,  $\hat{H}$ ,  $\hat{H}_i$ , and  $\hat{H}_s(T)$  and the chemical production terms  $r_i$ ,  $r_{hs}$  and  $r_s$  are written in terms of their respective mole quantities to give the pyrolysis gas energy equation in terms of mole quantities as

$$\begin{aligned}
\eta \sum_i \frac{\rho_i C_{pi}}{M_i} \frac{DT}{Dt} = & - \eta \left( \frac{\partial \ln \rho}{\partial \ln T} \right)_{P, x_i} \frac{DP}{Dt} - \eta \sum_i H_i R_{Ti} \\
& + \sum_i H_i \vec{\nabla} \cdot \vec{J}_i + P \frac{D\eta}{Dt} + \frac{1}{2} \eta v^2 \sum_i R_{Ti} M_i \\
& + \eta \bar{\tau} : \vec{\nabla} \vec{v} + \eta \sum_i \frac{\vec{J}_i}{M_i} \cdot \vec{g}_i - \vec{\nabla} \cdot \vec{q} + \eta (A' - \epsilon') \\
& + H_A (T_s - T) - \eta R_s H(T)_s - \eta R_{hs} H_s \\
& + \eta \sum_r r_h^{(r)} \Delta H^{(r)} .
\end{aligned} \tag{2-58}$$

Pyrolysis gas pressure differential equation.— The basic law governing the velocity of fluids flowing through porous media is the phenomenological law of Darcy which states that the rate of flow through porous media is directly proportional to the pressure gradient causing flow. Darcy's law written in equation form as in Scheidegger (Ref. 23) is

$$\vec{v}_o = - \frac{K}{\mu} \vec{\nabla} P \tag{2-59}$$

or

$$\vec{v} = - \frac{K}{\mu \eta} \vec{\nabla} P . \tag{2-60}$$

Equation 2-59 may be combined with the total mass conservation equation to give

$$\frac{\partial}{\partial t} (\eta \rho) - \vec{\nabla} \cdot \left( \frac{\rho K}{\mu} \vec{\nabla} P \right) - \eta \sum_i R_{T_i} M_i = 0. \quad (2-61)$$

The equation of state for the pyrolysis gases,

$$P = \rho R_u T / \bar{M} \quad (2-62)$$

and the identity

$$P \vec{\nabla} P = \frac{1}{2} \vec{\nabla} P^2 \quad (2-63)$$

are used in Eq. 2-61 to give the differential equation for pyrolysis gas pressure as

$$\begin{aligned} \vec{\nabla} \cdot \vec{\nabla} P^2 + \frac{\mu T}{K \bar{M}} \vec{\nabla} \left( \frac{K \bar{M}}{\mu T} \right) \cdot \vec{\nabla} P^2 \\ - \frac{2 \mu R_u T}{K \bar{M}} \left[ \frac{\partial}{\partial t} (\eta \rho) - \eta \sum_i R_{T_i} M_i \right] = 0. \end{aligned} \quad (2-64)$$

Chemical reaction rate equations.— The rate of chemical reactions occurring within the char layer must be computed using an appropriate chemistry model. The model considered here treats homogeneous and heterogeneous reactions. The rate of removal of chemical species by

homogeneous reactions is governed by the Law of Mass Action which states that the rate of removal of a chemical species is proportional to the product of the concentrations of the reacting species where each and every chemical species concentration is raised to a power equal to its stoichiometric coefficient. In equation form, the Law of Mass Action as written by Clarke and McChesney (Ref. 24) for a one-step chemical reaction described by the following stoichiometric relation



is

$$\text{reaction rate} = k \prod_i [A_i]^{\nu_i'}, \quad (2-66)$$

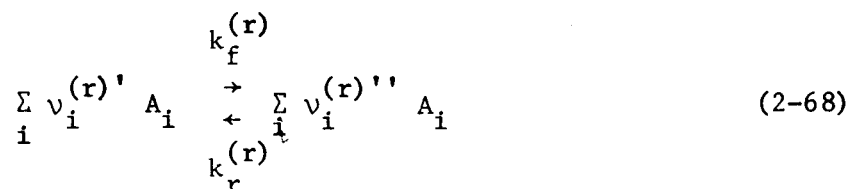
where the reaction rate constant  $k$  is considered to be independent of the concentration of chemical species and dependent on temperature. The reaction rate constant is given by

$$k = A T^S \exp (-B/T) \quad (2-67)$$

where  $A$  and  $B$  are the frequency factor and activation energy for the reaction.

Simultaneous forward and reverse chemical reactions are represented by





where

$r = 1, 2, \dots, m$  independent reactions.

The rate of forward reaction for the chemical reaction represented by the  $r^{\text{th}}$  equation is

$$\text{rate of forward reaction} = k_f^{(r)} \prod_i [A_i]^{v_i^{(r)'}} \quad (2-69)$$

and the rate of reverse reaction is

$$\text{rate of reverse reaction} = k_r^{(r)} \prod_i [A_i]^{v_i^{(r)''}} \quad (2-70)$$

Thus the net rate of progress of the  $r^{\text{th}}$  reaction in the forward direction is given by

$$r^{(r)} = k_f^{(r)} \prod_i [A_i]^{v_i^{(r)'}} - k_r^{(r)} \prod_i [A_i]^{v_i^{(r)'}} \quad (2-71)$$

Now this reaction yields a predetermined number of moles of chemical species  $i$  as indicated by the coefficients in the stoichiometric

representation of the chemical reaction. Therefore, the molar rate of production of chemical species  $i$  is given by

$$R_i = \sum_r [v_i^{(r)''} - v_i^{(r)'}] \{ k_f^{(r)} \prod_i [A_i]^{v_i^{(r)'}} - k_r^{(r)} \prod_i [A_i]^{v_i^{(r)'}} \} \quad (2-72)$$

Equations 2-69 and 2-70 are based on the Law of Mass Action and are general expressions for the forward and reverse reaction rates of some chemical reaction occurring in a gaseous system. Most frequently the chemical kinetics data for a particular reaction are based on empirical curve fits to experimental data. Such chemical kinetics data are usually presented with a rate law which best describes the particular chemical process.

The theory describing heterogeneous chemical reactions or reactions occurring at the gas-solid interface is somewhat more complicated than for homogeneous chemical reactions. It was assumed by Laidler (Ref. 25) that there are four steps involved in the interaction of the gas molecules with the solid phase. These steps are: (1) The reacting molecules diffuse to the solid surface. (2) The molecules are adsorbed on the surface. (3) The molecules undergo chemical reactions giving gaseous and or solid products. (4) The gaseous product molecules diffuse from the surface. The usual treatment of surface reactions is based on a concept due to Langmuir and Hinshelwood

which is discussed in Emmett (Ref. 26). The Langmuir-Hinshelwood mechanism assumes that the reactants are in adsorptive equilibrium with the solid surface. The reaction then involves the adsorbed molecules. Quantitative treatment of the reactions by this mechanism, therefore, involves obtaining an expression, using the adsorption isotherm, for the concentration of the reactant molecules on the surface. Thus, expressing the rate of reaction in terms of these surface concentrations, the rate of reaction can be expressed in terms of the concentrations of the gaseous reactants.

Following the development of Alekseyev (Ref. 27), the Law of Surface Action for the heterogeneous reaction



states that the rate of the process is proportional to the product of the portions of the surface occupied by reacting species raised to powers equal to the corresponding stoichiometric coefficients. In equation form

$$\text{reaction rate} = k \prod_j [\theta_j]^{\nu'_j} \theta_o^n \quad (2-74)$$

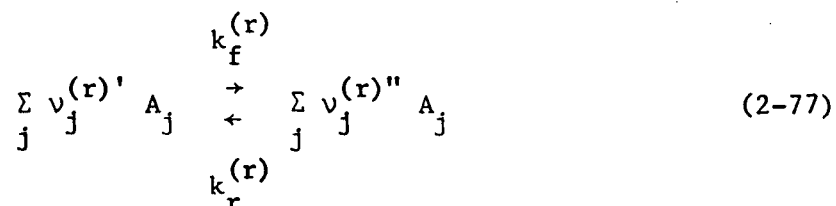
where the reaction rate constant is given by an equation of the form

$$k = A \exp (-B/T) \quad (2-75)$$

and

$$n = \sum_j (v_j'' - v_j') \quad (2-76)$$

Simultaneous forward and reverse heterogeneous chemical reactions are represented by



where  $r = 1, 2, \dots, m$  independent reactions. The rate of the forward reaction for the chemical reaction represented by the  $r^{\text{th}}$  equation is

$$\text{rate of forward reaction} = k_f^{(r)} \prod_j [\theta_j]^{v_j^{(r)'}} \theta_o^{n(r)} \quad (2-78)$$

and the rate of the reverse reaction is

$$\text{rate of reverse reaction} = k_r^{(r)} \prod_j [\theta_j]^{v_j^{(r)'}} \theta_o^{n(r)} \quad (2-79)$$

Thus the net rate of the  $r^{\text{th}}$  reaction is given by

$$r_h^{(r)} = \left\{ k_f^{(r)} \prod_j [\theta_j]^{v_j^{(r)'}} - k_r^{(r)} \prod_j [\theta_j]^{v_j^{(r)'}} \right\} \theta_o^{n(r)} A_s \quad (2-80)$$

and the molar rate of production of chemical species  $j$  resulting from the set of reactions (Eq. 2-77) is

$$R_{h,j} = \sum_r [v_j^{(r)''} - v_j^{(r)'}] \left\{ k_f^{(r)} \prod_j [\theta_j]^{v_j^{(r)'}} - k_r^{(r)} \prod_j [\theta_j]^{v_j^{(r)'}} \right\} A_s \theta_o^n(r) \quad (2-81)$$

where the factor  $A_s$  is the surface area per volume and is included to give rate of production per volume for heterogeneous chemical reactions occurring in porous media.

There is very little chemical kinetics data available for reactions and conditions of interest in the field of ablation. When data are available it is presented with a rate law which best describes the particular chemical reaction.

#### Uncharred Material and Substrate Insulation Equations

The single energy transfer mechanism occurring in the uncharred material and substrate insulation is heat transfer by conduction. Thus the differential equation governing the thermal behavior of these regions is the conduction equation given by

$$\vec{\nabla} \cdot k_s' \vec{\nabla} T_s' = \rho_s' \hat{C}_{p_s}' \frac{\partial T_s'}{\partial t} \quad (2-82)$$

and

$$\vec{\nabla} \cdot k_s'' \vec{\nabla} T_s'' = \rho_s'' \hat{C}_{p_s}'' \frac{\partial T_s''}{\partial t}, \quad (2-83)$$

respectively.

## CHAPTER III

### BOUNDARY CONDITIONS AND INITIAL CONDITIONS

This analysis refers to the stagnation point of a body, hence the governing equations derived in Chapter II are reduced to one dimension in space. The equations to be solved are:

Char Layer Equations.-

Char temperature

$$\begin{aligned}
 (1 - \eta) \frac{\rho_s C_{ps}}{M_s} \frac{\partial T_s}{\partial t} &= \frac{\partial}{\partial y} \left( k_s \frac{\partial T_s}{\partial y} \right) - H_A (T_s - T) \\
 &+ \eta R_s H(T)_s + \eta R_{hs} H_s - \eta \sum_r r_h^{(r)} \Delta H^{(r)} + (1 - \eta)(A - \epsilon) \\
 &+ (1 - \eta) q_s''' + \frac{\rho_s H_s}{M_s} \frac{\partial \eta}{\partial t}
 \end{aligned} \tag{3-1}$$

Char porosity

$$\frac{\partial \eta}{\partial t} = - \eta \frac{M_s}{\rho_s} (R_{hs} + R_s) \tag{3-2}$$

Pyrolysis gas temperature

$$\begin{aligned}
 \eta \sum_i \frac{\rho_i C_{pi}}{M_i} \left( \frac{\partial T}{\partial t} + v \frac{\partial T}{\partial y} \right) &= - \eta \left( \frac{\partial \ln \rho}{\partial \ln T} \right)_{P, x_i} \left( \frac{\partial P}{\partial t} \right. \\
 &+ v \frac{\partial P}{\partial y} \left. \right) - \eta \sum_i H_i R_{Ti} + \sum_i H_i \frac{\partial}{\partial y} J_i + P \frac{\partial \eta}{\partial t} + P v \frac{\partial \eta}{\partial y}
 \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} \eta v^2 \sum_i R_{T_i} M_i + \eta \bar{\tau}_{yy} \frac{\partial v}{\partial y} + \eta \sum_i \frac{J_i g_i}{M_i} - \frac{\partial}{\partial y} q_y \\
& + \eta (A' - \epsilon') + H_A (T_s - T) - \eta R_s H(T)_s - \eta R_{hs} H_s \\
& + \eta \sum_r r_h^{(r)} \Delta H(r) \tag{3-3}
\end{aligned}$$

Chemical species continuity equation

$$\frac{\partial}{\partial t} (\eta \rho_i) + \frac{\partial}{\partial y} (\rho_i v_o) + \frac{\partial}{\partial y} \eta j_i - \eta r_{T_i} = 0 \tag{3-4}$$

Total mass conservation equation

$$\frac{\partial}{\partial t} (\eta \rho) + \frac{\partial}{\partial y} (\rho v_o) - \eta \sum_i r_{T_i} = 0 \tag{3-5}$$

Pressure of pyrolysis gas

$$\begin{aligned}
& \frac{\partial^2 P^2}{\partial y^2} + \frac{\mu T}{K\bar{M}} \frac{\partial}{\partial y} \left( \frac{K\bar{M}}{\mu T} \right) \frac{\partial P^2}{\partial y} - \frac{2\mu R_u T}{K\bar{M}} \left[ \frac{\partial}{\partial t} (\eta \rho) \right. \\
& \left. - \eta \sum_i R_{T_i} M_i \right] = 0 \tag{3-6}
\end{aligned}$$

Uncharred Layer and Substrate Insulation Equations.-

Uncharred layer temperature

$$\frac{\partial}{\partial y} \left( k'_s \frac{\partial T'_s}{\partial y} \right) = \rho'_s \hat{C}_{p'_s} \frac{\partial T'_s}{\partial t} \tag{3-7}$$

### Substrate insulation temperature

$$\frac{\partial}{\partial y} \left( k_s'' \frac{\partial T_s''}{\partial y} \right) = \rho_s'' \hat{C}_{p_s}'' \frac{\partial T_s''}{\partial t} . \quad (3-8)$$

It is convenient to treat the equations for char temperature, uncharred layer temperature and substrate insulation temperature as a set of coupled equations. That is, the char temperature equations are related to the uncharred layer temperature equation through the boundary condition at the char-uncharred interface. The equations for the uncharred layer and the insulation layer are similarly related. From this point forward, reference to the solid temperature will mean the temperature of the particular layer of interest.

### Solid Temperature Equations

Two conditions must be specified at the front surface of the char layer. The first condition is an expression for the rate of material removal or the surface temperature and the second is an energy balance.

Surface removal by oxidation.— There are two regimes of surface removal by oxidation. The first regime is the rate controlled regime. The rate of surface removal by oxidation is rate controlled when conditions of temperature and pressure are low enough that the rate of oxygen consumption in the chemical process does not exceed the rate of oxygen diffusion through the boundary layer to the surface. As the surface temperature and pressure increase, the rate of surface removal



goes through a transition from the rate controlled regime to a diffusion controlled regime. In the diffusion controlled regime, surface removal by oxidation depends on the rate of oxygen diffusion to the surface. Nolan and Scala (Ref. 28) express the rate of surface removal by oxidation in the rate controlled regime in terms of chemical kinetics, writing the mass loss rate as

$$\dot{m}_s = k (P_{O_2})_w^n \quad (3-9)$$

where the exponent  $n$  is the order of the reaction. The specific reaction rate is obtained from

$$k = A_s \exp(-B_s/T_{s1}). \quad (3-10)$$

The oxygen partial pressure at the wall may be written in terms of the mass fraction of oxygen as follows:

$$(P_{O_2})_w = (x_{O_2})_w P_e \quad (3-11)$$

$$P_w = P_e \quad (3-12)$$

$$(x_{O_2})_w = C_w \bar{M}_w / M_{O_2} \quad (3-13)$$

Therefore,

$$(P_{O_2})_w = \frac{C_w \bar{M}_w}{M_{O_2}} P_e . \quad (3-14)$$

Equations 3-9, 3-10, and 3-14 are combined to give the rate of surface removal by rate controlled oxidation as

$$\dot{m}_s = A_s \exp(-B_s/T_{s1}) \left( \frac{C_w \bar{M}_w}{M_{O_2}} P_e \right)^n . \quad (3-15)$$

In subsonic and supersonic flow, the stagnation pressure is given by the solution of the inviscid flow problem. The stagnation pressure in hypersonic flow is approximated in Truitt (Ref. 29) by

$$P_{w,s} = \frac{11}{12} \rho_e v_e^2 . \quad (3-16)$$

In Ref. 30 Chapman relates the heating rate and enthalpy to the free stream conditions by

$$q_c \propto \sqrt{\rho_e / \text{Rad}} v_e^3 \quad (3-17)$$

and

$$\hat{H}_e \propto v_e^2 . \quad (3-18)$$

Thus the wall pressure is approximated by

$$P_{w,s} = 5.693 \times 10^6 \text{ Rad } (q_c/\hat{H}_e)^2 . \quad (3-19)$$

In the current problem,

$$P_w = P_{w,s} \quad (3-20)$$

thus

$$P_w = 5.693 \times 10^6 \text{ Rad } (q_c/\hat{H}_e)^2 . \quad (3-21)$$

In the diffusion controlled regime, surface removal by oxidation depends on the rate of oxygen diffusion to the surface as expressed in the following equation

$$\dot{m}_s = \lambda \dot{m}_{O_2} \quad (3-22)$$

where  $\lambda$  is the ratio of the mass of char layer removed by oxidation to the mass of oxygen diffusing to the surface.

In Ref. 10 Swann presents an analysis of oxidation of carbon surfaces near the stagnation region of a body in a nonreacting mixture of two gases having the same specific heats. Following Swann's development, the boundary layer equation for conservation of oxygen is

$$\bar{\rho} u \frac{\partial C}{\partial z} + \bar{\rho} v \frac{\partial C}{\partial y} = \frac{\partial}{\partial y} \left( \frac{\mu}{N_{Sc}} \frac{\partial C}{\partial y} \right) \quad (3-23)$$

and the boundary layer energy equation is

$$\bar{\rho} u \frac{\partial \hat{H}}{\partial z} + \bar{\rho} v \frac{\partial \hat{H}}{\partial y} = \frac{\partial}{\partial y} \left[ \frac{\mu}{N_{Pr}} \frac{\partial \hat{H}}{\partial y} + \frac{\mu}{2} \left( 1 - \frac{1}{N_{Pr}} \right) \frac{\partial u^2}{\partial y} \right]. \quad (3-24)$$

Equations 3-21 and 3-22 are formally similar if  $N_{Pr} = 1$  or if  $\frac{\partial u^2}{\partial y}$  is small relative to  $\frac{\partial \hat{H}}{\partial y}$ , which is valid at stagnation regions. Also, the boundary conditions for these two equations are identical, that is

$$\left. \begin{array}{l} C = C_w \\ \hat{H} = \hat{H}_w \end{array} \right\} \text{ at } y = 0 \quad (3-25)$$

and

$$\left. \begin{array}{l} C = C_e \\ \hat{H} = \hat{H}_e \end{array} \right\} \text{ at } y = \infty. \quad (3-26)$$

Nondimensionalizing Eqs. 3-23 and 3-24 with

$$\left. \begin{aligned} \bar{C} &= \frac{C - C_w}{C_e - C_w} \\ \bar{H} &= \frac{\hat{H} - \hat{H}_w}{\hat{H}_e - \hat{H}_w} \end{aligned} \right\} \quad (3-27)$$

gives

$$\left. \begin{aligned} \bar{\rho} u \frac{\partial \bar{C}}{\partial z} + \bar{\rho} v \frac{\partial \bar{C}}{\partial y} &= \frac{\partial}{\partial y} \frac{\mu}{N_{sc}} \frac{\partial \bar{C}}{\partial y} \\ \bar{\rho} u \frac{\partial \bar{H}}{\partial z} + \bar{\rho} v \frac{\partial \bar{H}}{\partial y} &= \frac{\partial}{\partial y} \frac{\mu}{N_{pr}} \frac{\partial \bar{H}}{\partial y} \\ \bar{C} = \bar{H} &= 0 \text{ at } y = 0 \\ \bar{C} = \bar{H} &= 1 \text{ at } y = \infty . \end{aligned} \right\} \quad (3-28)$$

Therefore, the solutions of the oxygen conservation equation and the energy conservation equation are formally similar. If the solution of the boundary layer energy equation is

$$\bar{H} = F_1(z, y, N_{pr}) \quad (3-29)$$

then the solution of the oxygen conservation equation is

$$\bar{C} = F_1(z, y, N_{sc}) . \quad (3-30)$$

The rate of oxygen transfer to the surface by diffusion may be expressed as

$$\dot{m}(O_2) = (C_e - C_w) \left( \frac{\mu}{N_{Sc}} \frac{\partial \bar{C}}{\partial y} \right)_w \quad (3-31)$$

and the rate of energy transfer to the surface may be expressed as

$$q = (H_e - H_w) \left( \frac{\mu}{N_{Pr}} \frac{\partial \bar{H}}{\partial y} \right)_w \quad (3-32)$$

Fay and Riddell (Ref. 31) show that the rate of energy transfer to the surface may be expressed as

$$q_{c,net} = 0.76 N_{Pr}^{-0.6} (\rho_w \mu_w)^{0.1} (\rho_s \mu_s)^{0.4} (\hat{H}_e - \hat{H}_w) \sqrt{\frac{du_e}{dz}} \quad (3-33)$$

Therefore, the rate of oxygen diffusion to the surface is

$$\dot{m}_{O_2} = 0.76 N_{Sc}^{-0.6} (\rho_w \mu_w)^{0.1} (\rho_s \mu_s)^{0.4} (C_e - C_w) \sqrt{\frac{du_e}{dz}} \quad (3-34)$$

Equations 3-33 and 3-34 are combined to give the rate of oxygen diffusion to the surface in terms of the energy transfer rate as

$$\dot{m}_{O_2} = \frac{N_{Sc}^{-0.6} (C_e - C_w)}{N_{Pr}^{-0.6} (\hat{H}_e - \hat{H}_w)} q_{c,net} \quad (3-35)$$

or

$$\dot{m}_{O_2} = \frac{C_e - C_w}{H_e - H_w} N_{Le}^{0.6} \bar{M}_w q_{c,net} \quad (3-36)$$

The rate of surface removal by oxidation in terms of energy transfer rate is obtained upon combining Eqs. 3-22 and 3-36. Thus,

$$\dot{m}_s = \frac{C_e - C_w}{H_e - H_w} \lambda N_{Le}^{0.6} \bar{M}_w q_{c,net} \quad (3-37)$$

Equation 3-15 written for a reaction of order 1 is combined with Eq. 3-37 to give an equation for the rate of surface removal which does not contain the oxygen concentration at the wall. Thus,

$$\dot{m}_s = \frac{k P_e C_e \bar{M}_w}{M_{O_2} + \frac{k P_e (H_e - H_w)}{\lambda N_{Le}^{0.6} q_{c,net}}} \quad (3-38)$$

where

$$k = A_s \exp(-B_s/T_{s1}) \quad (3-39)$$

Front surface energy balance.— The second condition to be specified at the front surface is a surface energy balance. Energy transfer to the surface results from convective and radiative heating and combustion heating in the case of surface removal by oxidation. This energy is accommodated by blocking due to mass injection into the boundary layer, reradiation from the

surface, conduction to the interior, and sublimation of the char layer when the surface temperature reaches the sublimation temperature of the char material.

Figure 2 from Swann, Pittman and Smith (Ref. 16) shows the effect of mass injection into the boundary layer on energy transfer to the surface. The exact solution is from the boundary layer solution by Roberts (Ref. 6) for air-to-air injection. The linear approximation is

$$q_{c,net} = q_c (1 - H_w/H_e) [1 - \bar{\eta} \dot{m}_T \hat{H}_e/q_c] \quad (3-40)$$

where

$$\dot{m}_T = \alpha_c \dot{m}_s + \alpha_p \dot{m}_l \quad (3-41)$$

and  $\bar{\eta} = 0.6$ . The second-order approximation, which was obtained by fitting a curve through points at  $\dot{m}_T \hat{H}_e/q_c = 0, 1.0$ , and  $2.5$  is

$$q_{c,net} = q_c (1 - H_w/H_e) \{1 - [.724 \dot{m}_T \hat{H}_e/q_c - .13 (\dot{m}_T \hat{H}_e/q_c)^2]\} . \quad (3-42)$$

Figure 2 shows the linear approximation to be good for values of  $\dot{m}_T \hat{H}_e/q_c \leq 1$ . The second-order approximation is good for  $\dot{m}_T \hat{H}_e/q_c < 2.25$ . In Ref. 16 Swann, Pittman and Smith specify a minimum value of



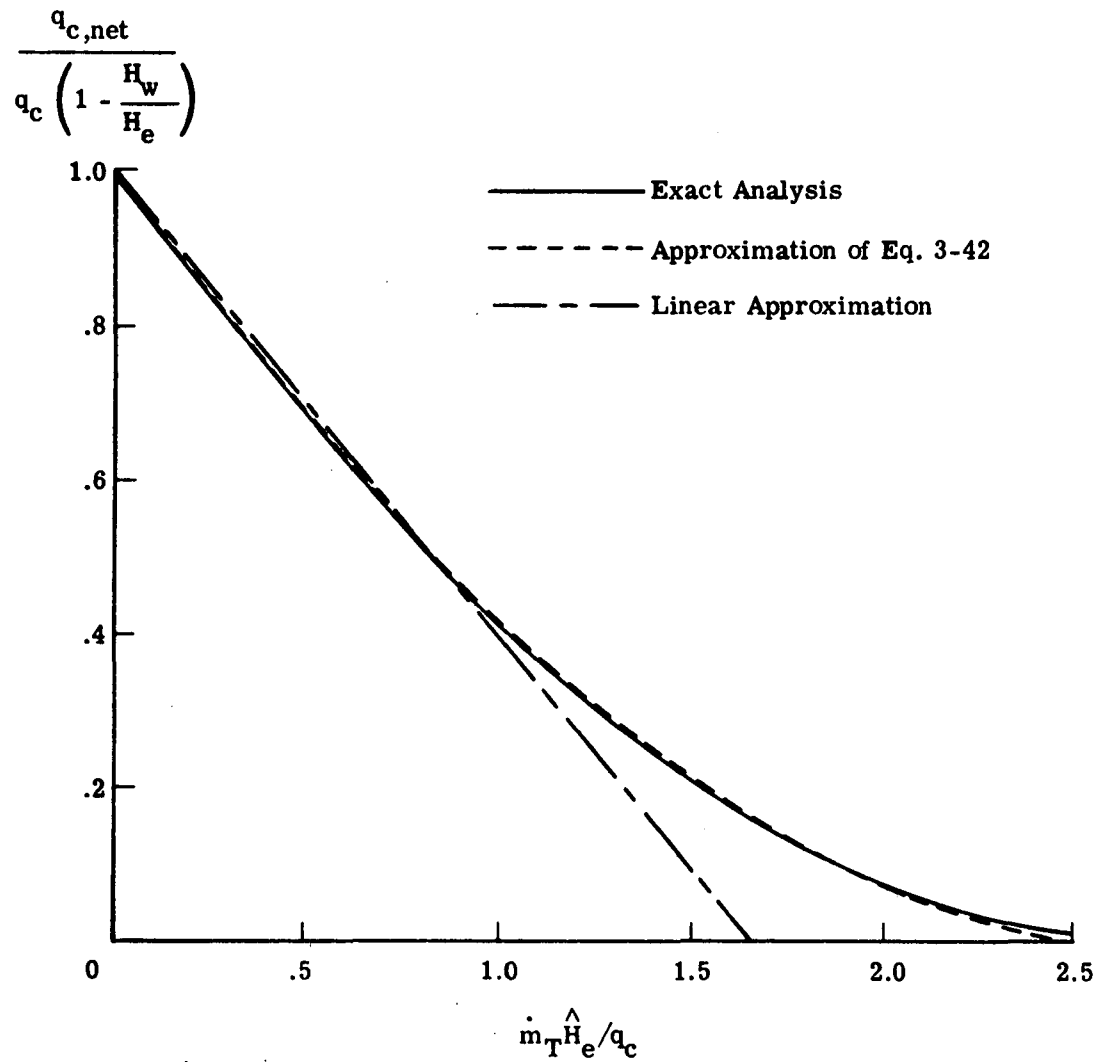


Figure 2.- Blocking effectiveness for a laminar boundary layer with air-to-air injection.

$\frac{q_{c,net}}{q_c(1 - H_w/H_e)}$  of 0.04 at  $\dot{m}_T \hat{H}_e / q_c = 2.25$ , where the second order curve departs the exact curve.

Writing the surface energy balance in equation form (Ref. 16)

$$q_c (1 - H_w/H_e) \{ 1 - (1 - \beta) [0.724 \dot{m}_T \hat{H}_e / q_c] \}$$

Cold Wall Convective Heating Rate      Hot-wall correction      Aerodynamic

← Net Convective

$$-0.13 (\dot{m}_T \hat{H}_e / q_c)^2 - \beta \bar{\eta} \dot{m}_T H_e / q_c \} + \alpha q_R$$

Blocking ----- Radiative Heating Rate

Heating →

$$+ [1 - S(T_{s1} - \bar{T}_1)] \dot{m}_s \Delta H_c = \sigma \epsilon_s T_{s1}^4$$

Combustion Heating Rate      Reradiation

$$- k_s \frac{\partial T_s}{\partial y} + S(T_{s1} - \bar{T}_1) \dot{m}_s H_c \quad (3-43)$$

Conduction to Interior      Heat of Sublimation of Char

where

$$\beta = 1 \text{ when } \dot{m}_T \hat{H}_e / q_c \leq 1.0$$

$$\beta = 0 \text{ when } \dot{m}_T \hat{H}_e / q_c > 1.0$$

$S(T_{s_1} - \bar{T}_1)$  is a step function defined by

$$S(T_{s_1} - \bar{T}_1) = 1 \text{ when } T_{s_1} = \bar{T}_1$$

$$S(T_{s_1} - \bar{T}_1) = 0 \text{ when } T_{s_1} < \bar{T}_1.$$

When the surface temperature is less than the sublimation temperature, Eq. 3-43 is solved for the temperature gradient at the surface  $\frac{\partial T_s}{\partial y}$  which is used as a boundary condition for solving the char temperature equation.

When the temperature of the char layer surface equals the sublimation temperature of the char material, the specified sublimation temperature of the material is used as a boundary condition and Eq. 3-43 is used to compute the rate of surface removal by sublimation.

Pyrolysis zone energy balance.— The second boundary condition to be specified for the char temperature equation is at the interface of the char layer and the uncharred layer. This equation is just an expression of conservation of energy at the interface energy conducted from the char layer to the interface is accommodated by pyrolysis reactions and conduction into the uncharred layer. In equation form

$$- \left( k_s \frac{\partial T_s}{\partial y} \right)_I = \dot{m}_g \Delta H_p - \left( (k'_s \frac{\partial T'_s}{\partial y})_I \right) . \quad (3-44)$$

Also, the temperature of the char layer equals the temperature of the uncharred layer at their interface.

$$T_{s_I} = T'_{s_I} . \quad (3-45)$$

Rate of pyrolysis of uncharred material.— The pyrolysis rate at the interface is given by an Arrhenius equation as follows:

$$\dot{m}_g = A' \exp (-B'/T_{s_I}) . \quad (3-46)$$

It is sometimes desirable to limit the temperature at the pyrolysis zone to some value  $\bar{T}_I$ . When such a restriction is used Eqs. 3-44 and 3-46 are employed as described until the pyrolysis zone temperature reaches  $\bar{T}_I$ , then Eq. 3-44 is used to determine the rate of pyrolysis of the uncharred layer and the boundary condition for  $T_s$  at the pyrolysis zone becomes  $T_{s_I} = \bar{T}_I$ .

Energy balance at the uncharred material-insulation interface.—

The boundary condition at the interface of the char layer and the uncharred layer also satisfies one of the requirements of the uncharred temperature equation for boundary conditions. The other boundary condition for the uncharred temperature equations results from an expression of conservation of energy at the interface of the uncharred

layer and the insulation layer--energy conducted from the uncharred layer to the surface is accommodated by energy conduction into the insulation and by increasing the temperature of the heat sink at the interface. In equation form

$$- \left( k'_s \frac{\partial T'_s}{\partial y} \right)_{I+J} = - \left( k''_s \frac{\partial T''_s}{\partial y} \right)_{I+J} + \rho_{Hs} \hat{C}_{p_{Hs}} \ell_{Hs} \left( \frac{\partial T'_s}{\partial t} \right)_{I+J} \quad (3-47)$$

Also the temperatures of the two layers are equal at their interface.

Thus

$$T'_s \text{ I + J } = T''_s \text{ I + J } \quad (3-48)$$

Back surface energy balance.— Equation 3-47 satisfies one of the requirements of the insulation temperature equation for boundary conditions. The other boundary condition for the insulation temperature equation results from an energy balance at the back surface--energy transfer to the back surface (conduction through the insulation plus energy transfer to the surface from the surroundings) is accommodated by energy radiation to the surroundings and by increasing the temperature of the heat sink at the back surface. In equation form

$$\begin{aligned} - \left( k''_s \frac{\partial T''_s}{\partial y} \right)_{I+J+K} + q_B &= \sigma \epsilon''_s T''_s{}^4 \text{ I + J + K } \\ &+ \rho_{HSP} \hat{C}_{p_{HSP}} \ell_{HSP} \left( \frac{\partial T''_s}{\partial t} \right)_{I+J+K} \quad (3-49) \end{aligned}$$

The effect of an adiabatic surface is achieved by setting the rate of energy transfer to the surface from the surroundings equal to the rate of energy radiated by the surface to the surroundings. Thus, for an adiabatic back surface

$$q_B = \sigma \epsilon_s'' T_s''^4 I + J + K . \quad (3-50)$$

Initial conditions.— Initially, the complete system is at a specified temperature; thus the initial condition for the solid phase temperature is

$$T_s(y, t) = T_{s_0}(y) \text{ at } t = 0 \quad (3-51)$$

where the superscript on  $T_s$  is neglected.

#### Char Porosity Equation

A single boundary condition is required for solution of the char layer porosity equation. The condition used in this analysis is a specified porosity of the char layer at the pyrolysis interface. The initial condition for the char layer porosity is

$$\eta(y, t) = \eta_0(y) \text{ at } t = 0. \quad (3-52)$$

#### Pyrolysis Gas Temperature Equation

The pyrolysis gas temperature equation requires a single boundary

condition. The condition employed is that the pyrolysis gas temperature is equal to the solid phase temperature at the pyrolysis zone. The initial condition for the pyrolysis gas temperature is

$$T(y,t) = T_o(y) \text{ at } t = 0. \quad (3-53)$$

#### Pyrolysis Gas Pressure Equation

The pyrolysis gas pressure distribution equation requires two boundary conditions.

Specified pressure at the front surface.— The first boundary condition is that the pressure is specified at the surface,

$$P_1 = P_w. \quad (3-54)$$

Specified pressure gradient at the pyrolysis zone.— The second is that the pressure gradient is specified at the interface. In developing the governing differential equation for pyrolysis gas pressure in Chapter II, Darcy's law was used to determine the superficial velocity of the pyrolysis gases in the char layer. In equation form, Darcy's law for a one-dimensional system is

$$v_o = - \frac{K}{\mu} \frac{\partial P}{\partial y} \quad (3-55)$$

Equation 3-55 is multiplied by  $\rho$  and the equation of state is used to give

$$\rho v_o = - \frac{K\bar{M}}{\mu R_u T} P \frac{\partial P}{\partial y} . \quad (3-56)$$

Equation 3-56 is applied at the pyrolysis zone and use is made of the equation

$$(\rho v_o)_I = - \dot{m}_g \quad (3-57)$$

to obtain

$$\left( \frac{\partial P}{\partial y} \right)_I = R_u \left( \frac{\mu T}{K\bar{M}P} \right)_I \dot{m}_g . \quad (3-58)$$

But

$$\frac{\partial P}{\partial y} = \frac{1}{2P} \frac{\partial P^2}{\partial y} \quad (3-59)$$

therefore

$$\left( \frac{\partial P^2}{\partial y} \right)_I = 2 R_u \left( \frac{\mu T}{K\bar{M}} \right)_I \dot{m}_g . \quad (3-60)$$



Initial conditions.— The initial condition for the pyrolysis gas pressure is

$$P(y,t) = P_{w,0} \text{ at } t = 0. \quad (3-61)$$

#### Total Mass Conservation Equation

The mass conservation equation is solved for the product  $\rho v_o$ , or the local mass flow rate. It requires a single boundary condition. The boundary condition used is that the mass flow rate is known at the pyrolysis interface, or in equation form

$$(\rho v_o)_I = -\dot{m}_g. \quad (3-62)$$

The initial condition for the mass flow rate is

$$(\rho v_o)_{y,t} = -\dot{m}_o(y) \text{ at } t = 0. \quad (3-63)$$

#### Chemical Species Conservation Equation

The chemical species continuity equation is solved for the local mass flow rate of each chemical species. It requires a single boundary condition. The boundary condition is obtained from the molar composition of the pyrolysis gases which is specified at the pyrolysis interface and the total pyrolysis gas flow rate at that point. This

boundary condition is expressed in equation form as

$$(\rho_i v)_I = - \left( \frac{x_i}{\eta M} \right)_I \dot{M}_i m_g . \quad (3-64)$$

The initial condition for the species continuity equation is

$$(\rho_i v)_{y,t} = (\rho_i v)_{y,o} \text{ at } t = 0. \quad (3-65)$$

## CHAPTER IV

### TRANSFORMATION AND LINEARIZATION OF EQUATIONS AND BOUNDARY CONDITIONS

The governing equations and boundary conditions presented to this point are for a physical system with boundaries which move relative to each other and relative to a fixed coordinate system. In maintaining a fixed number of stations in layers of varying thickness when obtaining a numerical solution to an equation it is necessary to interpolate after each iteration as the location of the stations change. Each such operation introduces a small error. This problem can be eliminated by transforming to a moving coordinate system in which the locations of the stations remain fixed and the coordinate system moves to accommodate changes in the location of the boundaries. The transformations presented by Swann, Pittman and Smith in Ref. 16 will be employed here. The location of the system boundaries with the new coordinate system is shown in Fig. 3. The finite char layer of thickness  $\ell_0$  at time  $t = 0$  is required for obtaining a numerical solution to the governing equations.

The equations and boundary conditions for the char layer are transformed to a coordinate system with the origin attached to the front surface. The dimensional moving coordinate system with the origin attached to the front surface results from the following transformation

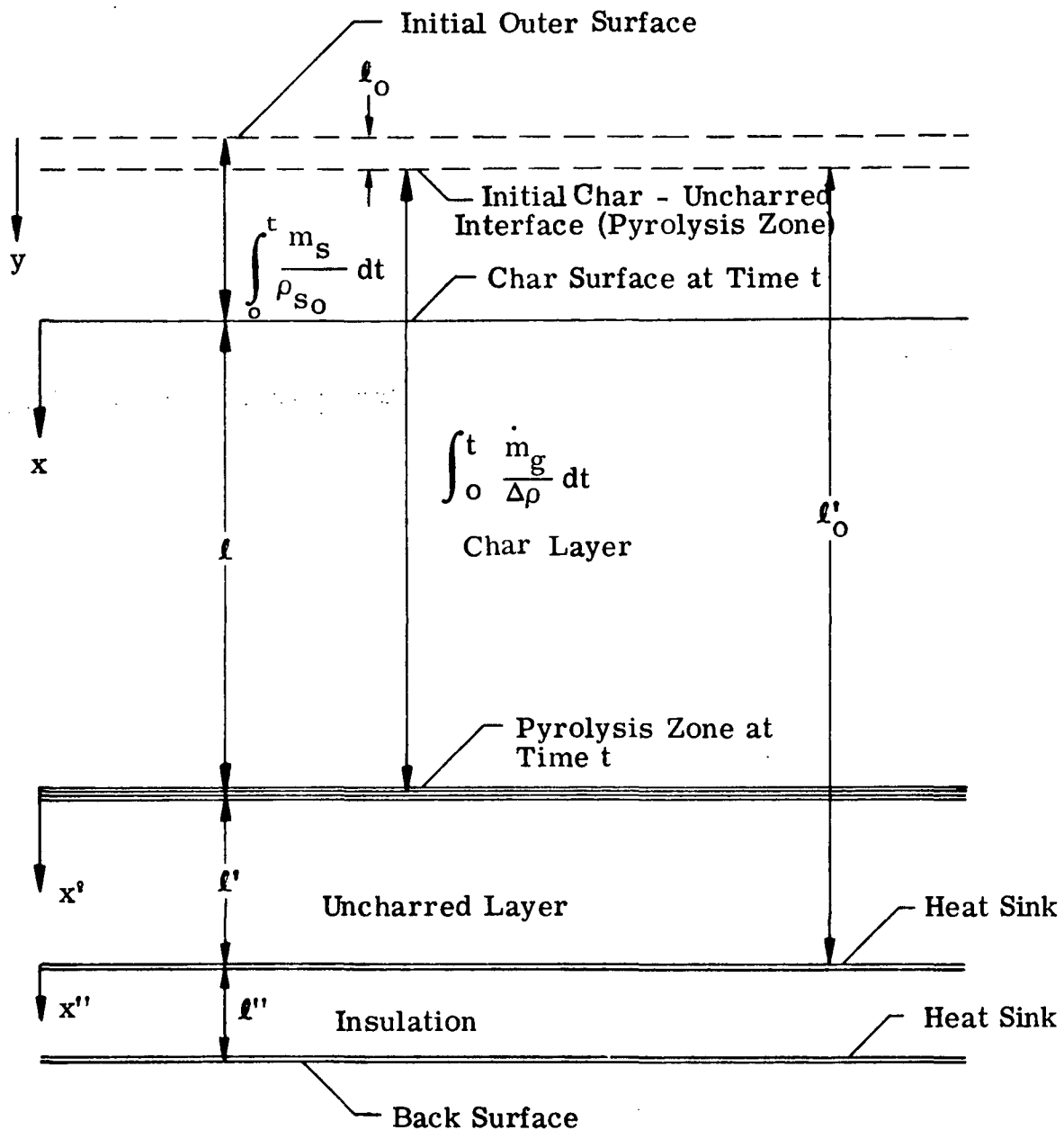


Figure 3.- Location of system boundaries and coordinates.

$$x_d = y - \int_0^t \frac{\dot{m}_s}{\rho_{s_0}} dt \quad (4-1)$$

where the integral represents the total surface recession at some time  $t$ . Equation 4-1 is nondimensionalized by the char layer thickness  $\ell$  to give the transformed dimensionless coordinate for the char layer as

$$x = \frac{y - \int_0^t \frac{\dot{m}_s}{\rho_{s_0}} dt}{\ell} \quad (4-2)$$

Note that the new coordinate system for the char layer is attached to the char layer surface and extends to the pyrolysis zone. The coordinates of the front surface and pyrolysis zone are constant at  $x = 0$  and  $x = 1$  respectively.

Similarly, the governing equations and boundary conditions for the uncharred layer are transformed to a moving coordinate system with the origin attached to the pyrolysis zone. The dimensional moving coordinate system with the origin attached to the pyrolysis zone results from the following transformation

$$x'_d = y - \ell_0 - \int_0^t \frac{\dot{m}_g}{\Delta \rho} dt \quad (4-3)$$

where  $\ell_0$  is the finite char thickness at time  $t = 0$  and the integral represents the thickness of uncharred material which has been degraded at some time  $t$ . Equation 4-3 is nondimensionalized by the uncharred material thickness  $\ell'$  to give the transformed dimensionless coordinate for the uncharred layer as

$$x' = \frac{y - \ell_o - \int_0^t \dot{m}_g / \Delta \rho \, dt}{\ell'} \quad (4-4)$$

Note that the new coordinate system for the uncharred layer is attached to the pyrolysis zone and extends to the uncharred material - insulation layer interface. The coordinates of the uncharred layer boundaries are  $x' = 0$  and  $x' = 1$ .

The boundaries of the insulation layer are fixed so the new coordinate system is stationary with the origin at the boundary between the uncharred layer and the insulation. The new coordinate system for the insulation layer results from transforming the initial system by an amount equal to the total initial thickness of the char layer and the uncharred layer and nondimensionalizing the result by the thickness of the insulation layer. In equation form

$$x'' = \frac{y - (\ell_o + \ell'_o)}{\ell''} \quad (4-5)$$

The coordinates of the insulation boundaries are  $x'' = 0$  and  $x'' = 1$ .

#### Char Layer Equations

Equation 4-2 is used to transform the governing equations for the char layer. The following derivative expressions are obtained:

$$\left( \frac{\partial}{\partial t} \right)_{\text{old}} = \left( \frac{\partial}{\partial t} \right)_{\text{New}} + \left[ \frac{\partial x}{\partial y} \frac{\partial y}{\partial t} + \frac{\partial x}{\partial \ell} \frac{\partial \ell}{\partial t} + \frac{\partial x}{\partial t} \right] \frac{\partial}{\partial x} \quad (4-6)$$

but

$$\left. \begin{aligned}
 \frac{\partial x}{\partial y} &= \frac{1}{\ell} \\
 \frac{\partial x}{\partial \ell} &= -x/\ell \\
 \frac{\partial x}{\partial t} &= -\frac{1}{\ell} \dot{m}_s / \rho_{s_o} \\
 \ell &= \ell_o + \int_0^t [\dot{m}_g / \Delta \rho - \dot{m}_s / \rho_{s_o}] dt \\
 \frac{\partial \ell}{\partial t} &= \dot{m}_g / \Delta \rho - \dot{m}_s / \rho_{s_o} .
 \end{aligned} \right\} \quad (4-7)$$

Therefore

$$\left( \frac{\partial}{\partial t} \right)_{old} = \left( \frac{\partial}{\partial t} \right)_{New} - v_c \frac{\partial}{\partial x} \quad (4-8)$$

where

$$v_c = \frac{1}{\ell} [\dot{m}_s / \rho_{s_o} + x(\dot{m}_g / \Delta \rho - \dot{m}_s / \rho_{s_o})] . \quad (4-9)$$

Also

$$\frac{\partial}{\partial y} = \frac{\partial x}{\partial y} \frac{\partial}{\partial x} \quad (4-10)$$

or

$$\frac{\partial}{\partial y} = \frac{1}{\ell} \frac{\partial}{\partial x} \quad (4-11)$$

and

$$\frac{\partial^2}{\partial y^2} = \frac{1}{\ell^2} \frac{\partial^2}{\partial x^2} \quad (4-12)$$

Char temperature equation.— Using these derivative expressions the char temperature equation becomes

$$\begin{aligned} (1 - \eta) \frac{\rho_s C_{ps}}{M_s} \left[ \frac{\partial T_s}{\partial t} - v_c \frac{\partial T_s}{\partial x} \right] &= \frac{k_s}{\ell^2} \frac{\partial^2 T_s}{\partial x^2} + \frac{1}{\ell^2} \frac{\partial k_s}{\partial x} \frac{\partial T_s}{\partial x} \\ &- H_A (T_s - T) + \eta R_s H(T)_s + \eta R_{hs} H_s - \eta \sum_r r_h^{(r)} \Delta H^{(r)} + (1 - \eta) (A - \epsilon) \\ &+ (1 - \eta) q_s''' + \frac{\rho_s H_s}{M_s} \left( \frac{\partial \eta}{\partial t} - v_c \frac{\partial \eta}{\partial x} \right) \quad (4-13) \end{aligned}$$

This equation can be written as

$$\frac{\partial^2 T_s}{\partial x^2} + \alpha_1 \frac{\partial T_s}{\partial x} + \alpha_2 T_s + \alpha_3 + \alpha_4 \frac{\partial T_s}{\partial t} = 0 \quad (4-14)$$

where



$$\alpha_1 = \frac{1}{k_s} \left[ \frac{\partial k_s}{\partial x} + \rho_s \ell^2 (1 - \eta) \frac{C_{ps}}{M_s} v_c \right] \quad (4-15)$$

$$\alpha_2 = - H_A \ell^2 / k_s \quad (4-16)$$

$$\begin{aligned} \alpha_3 = \frac{\ell^2}{k_s} \left[ H_A T + \eta R_s H(T)_s + \eta R_{hs} H_s - \eta \sum_r r_h^{(r)} \Delta H^{(r)} + (1 - \eta)(A - \epsilon) \right. \\ \left. + (1 - \eta) q_s''' + \frac{\rho_s H_s}{M_s} \left( \frac{\partial \eta}{\partial t} - v_c \frac{\partial \eta}{\partial x} \right) - \eta \sum_j R_{hj} \Delta H_j \right] \quad (4-17) \end{aligned}$$

$$\alpha_4 = - (1 - \eta) \ell^2 \rho_s C_{ps} / M_s k_s \quad (4-18)$$

The form of Eq. 4-12 is convenient for obtaining a solution by numerical methods. In obtaining a numerical solution to Eq. 4-12 the  $\alpha$ 's are considered to be independent of  $T_s$ , thus Eq. 4-12 becomes linear.

Char porosity equation.— The transformed char layer porosity equation is

$$\frac{\partial \eta}{\partial t} - v_c \frac{\partial \eta}{\partial x} + \eta \frac{M_s}{\rho_s} (R_{hs} + R_s) = 0 \quad (4-19)$$

or, writing it in the linear form,

$$\frac{\partial \eta}{\partial x} + \epsilon_1 \eta + \epsilon_2 + \epsilon_3 \frac{\partial \eta}{\partial t} = 0 \quad (4-20)$$

where

$$\epsilon_1 = - \frac{M_s}{\rho_s} (R_{hs} + R_s) / V_c \quad (4-21)$$

$$\epsilon_2 = 0 \quad (4-22)$$

$$\epsilon_3 = 1/V_c \quad (4-23)$$

Pyrolysis gas temperature equation.— The transformed pyrolysis gas temperature equation is

$$\begin{aligned} \eta \sum_i \frac{\rho_i C_{pi}}{M_i} \left[ \frac{\partial T}{\partial t} + (v/\ell - v_c) \frac{\partial T}{\partial x} \right] &= - \eta \left( \frac{\partial \ln \rho}{\partial \ln T} \right)_{P, x_i} \left[ \frac{\partial P}{\partial t} \right. \\ &\quad \left. + (v/\ell - v_c) \frac{\partial P}{\partial x} \right] - \eta \sum_i H_i R_{T_i} + \sum_i H_i \frac{1}{\ell} \frac{\partial}{\partial x} J_i \\ &\quad + P \left[ \frac{\partial \eta}{\partial t} + (v/\ell - v_c) \frac{\partial \eta}{\partial x} \right] + \frac{1}{2} \eta v^2 \sum_i R_{T_i} M_i \\ &\quad + \eta / \ell^3 \tau_{xx} \frac{\partial v}{\partial x} + \eta \sum_i \frac{J_i g_i}{M_i} - \frac{1}{\ell} \frac{\partial}{\partial x} q_x \\ &\quad + \eta (A' - \epsilon') + H_A (T_s - T) - \eta R_s H(T)_s - \eta R_{hs} H_s \\ &\quad + \eta \sum_r r_h^{(r)} \Delta H^{(r)} . \end{aligned} \quad (4-24)$$

Since

$$\rho = \bar{P}\bar{M}/R_u T \quad (4-25)$$

$$\left( \frac{\partial \ln \rho}{\partial \ln T} \right)_{P, x_i} = -1 \quad (4-26)$$

Also

$$\frac{\partial P}{\partial T} = \sum_i \rho_i / M_i R_u \frac{\partial T}{\partial T} + R_u T \frac{\partial}{\partial T} \sum_i \rho_i / M_i \quad (4-27)$$

and

$$\frac{\partial P}{\partial x} = \sum_i \rho_i / M_i R_u \frac{\partial T}{\partial x} + R_u T \frac{\partial}{\partial x} \sum_i \rho_i / M_i \quad (4-28)$$

Therefore Eq. 4-24 can be written as

$$\begin{aligned} & \eta (v/\ell - v_c) \left[ \sum_i \frac{\rho_i C_{p_i}}{M_i} - R_u \sum_i \rho_i / M_i \right] \frac{\partial T}{\partial x} + \left\{ H_A \right. \\ & - \eta R_u \left[ \frac{\rho}{\eta \bar{M}} \left( \frac{\partial \eta}{\partial T} - v_c \frac{\partial \eta}{\partial x} \right) + \frac{\partial}{\partial T} \left( \sum_i \rho_i / M_i \right) \right. \\ & \left. \left. + (v/\ell - v_c) \frac{\partial}{\partial x} \left( \sum_i \rho_i / M_i \right) \right] \right\} T + \eta \sum_i H_i R_{T_i} \\ & - \frac{1}{\ell} \sum_i H_i \frac{\partial}{\partial x} J_i - \eta \frac{v^2}{2} \sum_i R_{T_i} M_i - \frac{\tau_{xx}}{\ell^3} \frac{\partial v}{\partial x} \\ & - \eta \sum_i \frac{J_i g_i}{M_i} + \frac{1}{\ell^2} \frac{\partial}{\partial x} q_x - \eta (A' - \epsilon') - H_A T_s \end{aligned}$$

$$\begin{aligned}
& + \eta R_s H(T)_s + \eta R_{hs} H_s - \eta \sum_r r_h^{(r)} \Delta H^{(r)} + \eta \left( \sum_i \frac{\rho_i c_{pi}}{M_i} \right. \\
& \left. - R_u \sum_i \rho_i / M_i \right) \frac{\partial T}{\partial t} = 0
\end{aligned} \tag{4-29}$$

or, in the linear form,

$$\frac{\partial T}{\partial x} + \beta_1 T + \beta_2 + \beta_3 \frac{\partial T}{\partial t} = 0 \tag{4-30}$$

where

$$\begin{aligned}
\beta_1 = \{ & H_A - \eta R_u \left[ \frac{\rho}{\eta M} \left( \frac{\partial \eta}{\partial t} - v_c \frac{\partial \eta}{\partial x} \right) + \frac{\partial}{\partial t} \left( \sum_i \rho_i / M_i \right) \right. \\
& \left. + (v/\ell - v_c) \frac{\partial}{\partial x} \left( \sum_i \rho_i / M_i \right) \right] \} / D1
\end{aligned} \tag{4-31}$$

$$D1 = \eta (v/\ell - v_c) \left[ \sum_i \frac{\rho_i c_{pi}}{M_i} - R_u \sum_i \rho_i / M_i \right] \tag{4-32}$$

$$\begin{aligned}
\beta_2 = & \left[ \eta \sum_i H_i R_{Ti} - \frac{1}{\ell} \sum_i H_i \frac{\partial}{\partial x} J_i - \eta \frac{v^2}{2} \sum_i R_{Ti} M_i \right. \\
& - \frac{\tau_{xx}}{\ell^3} \frac{\partial v}{\partial x} - \eta \sum_i \frac{J_i g_i}{M_i} + \frac{1}{\ell^2} \frac{\partial}{\partial x} q_x \\
& - \eta (A' - \epsilon') - H_A T_s + \eta R_s H(T)_s + \eta R_{hs} H_s \\
& \left. - \eta \sum_r r_h^{(r)} \Delta H^{(r)} \right] / D1
\end{aligned} \tag{4-33}$$

$$\beta_3 = \eta \left( \sum_i \frac{\rho_i C_{Pi}}{M_i} - R_u \sum_i \rho_i / M_i \right) / D1 \quad (4-34)$$

Chemical species continuity equation.— The transformed chemical species continuity equation is

$$\frac{\partial}{\partial t} (\eta \rho_i) - v_c \frac{\partial}{\partial x} (\eta \rho_i) + \frac{1}{\ell} \frac{\partial}{\partial x} (\rho_i v_o) + \frac{1}{\ell} \frac{\partial}{\partial x} \eta j_i - \eta R_{T_i} M_i = 0, \quad (4-35)$$

This equation is combined with the identities

$$\dot{m}_i = - \rho_i v \quad (4-36)$$

and

$$v_o = \eta v \quad (4-37)$$

to obtain

$$\begin{aligned} & \eta \left( \frac{v_c}{v} - \frac{1}{\ell} \right) \frac{\partial}{\partial x} \dot{m}_i + \left[ \left( \frac{v_c}{v} - \frac{1}{\ell} \right) \frac{\partial \eta}{\partial x} - \frac{\eta}{v^2} \frac{\partial v}{\partial x} \right. \\ & \left. - \frac{1}{v} \frac{\partial \eta}{\partial t} \right] \dot{m}_i + \frac{1}{\ell} \frac{\partial}{\partial x} \eta j_i - \eta R_{T_i} M_i + \eta \frac{\partial \rho_i}{\partial t} = 0 \end{aligned} \quad (4-38)$$

or, in linear form,

$$\frac{\partial \dot{m}_i}{\partial x} + \Delta_{1_i} \dot{m}_i + \Delta_{2_i} + \Delta_{3_i} \frac{\partial \dot{m}_i}{\partial t} = 0 \quad (4-39)$$

where

$$\Delta_{1_i} = \frac{1}{\eta} \frac{\partial \eta}{\partial x} + \left[ \frac{\eta R_{T_i} M_i}{\rho_i} - \eta \frac{V_c}{v} \frac{\partial v}{\partial x} - \frac{\partial \eta}{\partial t} \right] / D2 \quad (4-40)$$

$$D2 = \eta (V_c - \frac{v}{\ell}) \quad (4-41)$$

$$\Delta_{2_i} = v \left( \frac{1}{\ell} \frac{\partial}{\partial x} \eta j_i + \eta \frac{\partial \rho_i}{\partial t} \right) / D2 \quad (4-42)$$

$$\Delta_{3_i} = 0 \quad (4-43)$$

Total mass conservation equation.— The transformed total mass conservation equation is

$$\frac{\partial}{\partial t} (\eta \rho) - V_c \frac{\partial}{\partial x} (\eta \rho) + \frac{1}{\ell} \frac{\partial}{\partial x} (\rho v_o) - \eta \sum_i R_{T_i} M_i = 0. \quad (4-44)$$

This equation is combined with the identity

$$\dot{m} = - \rho v_o \quad (4-45)$$

to obtain

$$\begin{aligned} \frac{\partial}{\partial x} \dot{m} &= \ell \left[ \frac{\partial}{\partial t} (\eta \rho) - \eta \sum_i R_{T_i} M_i \right. \\ &\quad \left. - V_c \left( \eta \frac{\partial \rho}{\partial x} + \rho \frac{\partial \eta}{\partial x} \right) \right] \end{aligned} \quad (4-46)$$

It is convenient to integrate this equation numerically rather than use finite difference methods, hence, it is not expressed in the linear form. The solution to this equation is used with the total density obtained from the equation of state to determine the mass average velocity of the pyrolysis gases.

Pyrolysis gas pressure equation.— The transformed pyrolysis gas pressure equation is

$$\begin{aligned} \frac{\partial^2 P^2}{\partial x^2} + \frac{\mu T}{K\bar{M}} \frac{\partial}{\partial x} \left( \frac{K\bar{M}}{\mu T} \right) \frac{\partial}{\partial x} P^2 - 2 \frac{\mu R_u T}{K\bar{M}} \left[ \frac{\partial}{\partial t} (\eta \rho) \right. \\ \left. - v_c \frac{\partial}{\partial x} (\eta \rho) - \eta \sum_i R_{T_i} M_i \right] = 0. \end{aligned} \quad (4-47)$$

This equation is combined with the equation of state to give

$$\begin{aligned} \frac{\partial^2 P^2}{\partial x^2} + \frac{\mu}{K} \left[ \frac{T}{\bar{M}} \frac{\partial}{\partial x} \left( \frac{K\bar{M}}{\mu T} \right) + \frac{\eta v_c}{P} \right] \frac{\partial P^2}{\partial x} \\ - \frac{2\mu}{\bar{M}KP} \left[ \eta \left( \frac{\partial \bar{M}}{\partial t} - \frac{\bar{M}}{T} \frac{\partial T}{\partial t} \right) + \bar{M} \left( \frac{\partial \eta}{\partial t} \right. \right. \\ \left. \left. - v_c \frac{\partial \eta}{\partial x} \right) + \eta \left( \frac{\bar{M}}{T} \frac{\partial T}{\partial x} - v_c \frac{\partial \bar{M}}{\partial x} \right) \right] P^2 \\ + \frac{2\mu\eta}{K\rho} \sum_i R_{T_i} M_i - \frac{\mu\eta}{KP} \frac{\partial P^2}{\partial t} = 0 \end{aligned} \quad (4-48)$$

or, in the linear form,

$$\frac{\partial^2 P^2}{\partial x^2} + \gamma_1 \frac{\partial P^2}{\partial x} + \gamma_2 P^2 + \gamma_3 + \gamma_4 \frac{\partial P^2}{\partial t} = 0 \quad (4-49)$$

where

$$\gamma_1 = \frac{\mu}{K} \left[ \frac{T}{\bar{M}} \frac{\partial}{\partial x} \left( \frac{K\bar{M}}{\mu T} \right) + \frac{\eta v_c}{P} \right] \quad (4-50)$$

$$\begin{aligned} \gamma_2 = & - \frac{2\mu}{\bar{M}K\rho} \left[ \eta \left( \frac{\partial \bar{M}}{\partial t} - \frac{\bar{M}}{T} \frac{\partial T}{\partial t} \right) \right. \\ & \left. + \bar{M} \left( \frac{\partial \eta}{\partial t} - v_c \frac{\partial \eta}{\partial x} \right) + \eta \left( \frac{\bar{M}}{T} \frac{\partial T}{\partial x} - v_c \frac{\partial \bar{M}}{\partial x} \right) \right] \end{aligned} \quad (4-51)$$

$$\gamma_3 = \frac{2\mu\eta}{K\rho} \sum_i R_{T_i} M_i \quad (4-52)$$

$$\gamma_4 = - \frac{\mu\eta}{K\rho} \quad (4-53)$$

#### Uncharred Layer Equation

Equation 4-4 is used to transform the governing energy equation for the uncharred layer. The following derivative expressions are obtained:

$$\left( \frac{\partial}{\partial t} \right)_{\text{old}} = \left( \frac{\partial}{\partial t} \right)_{\text{New}} + \left[ \frac{\partial x'}{\partial y} \frac{\partial y}{\partial t} + \frac{\partial x'}{\partial \ell'} \frac{\partial \ell'}{\partial t} + \frac{\partial x'}{\partial t} \right] \frac{\partial}{\partial x} \quad (4-54)$$

but



$$\left. \begin{aligned}
 \frac{\partial x'}{\partial y} &= \frac{1}{\ell'} \\
 \frac{\partial x'}{\partial \ell'} &= -\frac{x'}{\ell'} \\
 \frac{\partial x'}{\partial t} &= -\frac{1}{\ell'} \dot{m}_g / \Delta \rho \\
 \ell' &= \ell'_0 - \int_0^t \dot{m}_g / \Delta \rho \, dt \\
 \frac{\partial \ell'}{\partial t} &= -\dot{m}_g / \Delta \rho
 \end{aligned} \right\} \quad (4-55)$$

Therefore

$$\left( \frac{\partial}{\partial t} \right)_{\text{old}} = \left( \frac{\partial}{\partial t} \right)_{\text{New}} + \frac{\dot{m}_g}{\Delta \rho} \left( \frac{x' - 1}{\ell'} \right) \frac{\partial}{\partial x'} \quad (4-56)$$

Also

$$\frac{\partial}{\partial y} = \frac{\partial x'}{\partial y} \frac{\partial}{\partial x'} \quad (4-57)$$

or

$$\frac{\partial}{\partial y} = \frac{1}{\ell'} \frac{\partial}{\partial x'} \quad (4-58)$$

and

$$\frac{\partial^2}{\partial y'^2} = \frac{1}{\ell'^2} \frac{\partial^2}{\partial x'^2} \quad (4-59)$$

These equations are employed to obtain the transformed energy equation for the uncharred layer as

$$\begin{aligned} \frac{k'_s}{\ell'^2} \frac{\partial^2 T_s}{\partial x'^2} + \left[ \frac{1}{\ell'^2} \frac{\partial k'_s}{\partial x'} + \frac{\rho'_s \hat{C}'_{ps} \dot{m}_g (1 - x')}{\ell' \Delta \rho} \right] \frac{\partial T_s}{\partial x'} \\ - \rho'_s \hat{C}'_{ps} \frac{\partial T_s}{\partial t} = 0 \end{aligned} \quad (4-60)$$

where the superscript on  $T_s$  is omitted. The linear form of this equation is

$$\frac{\partial^2 T_s}{\partial x'^2} + \alpha'_1 \frac{\partial T_s}{\partial x'} + \alpha'_2 T_s + \alpha'_3 + \alpha'_4 \frac{\partial T_s}{\partial t} = 0 \quad (4-61)$$

where

$$\alpha'_1 = \frac{1}{k'_s} \left[ \frac{\partial k'_s}{\partial x'} + \frac{\ell' \rho'_s \hat{C}'_{ps} \dot{m}_g (1 - x')}{\Delta \rho} \right] \quad (4-62)$$

$$\alpha'_2 = 0 \quad (4-63)$$

$$\alpha'_3 = 0 \quad (4-64)$$



$$\alpha_4' = - \rho_s' \hat{C}_{p_s}' \ell'^2 / k_s' . \quad (4-65)$$

### Insulation Layer Equation

Equation 4-5 is used to transform the governing energy equation for the insulation layer. The following derivative expressions are obtained:

$$\left( \frac{\partial}{\partial t} \right)_{\text{Old}} = \left( \frac{\partial}{\partial t} \right)_{\text{New}} \quad (4-66)$$

$$\frac{\partial}{\partial y} = \frac{\partial x''}{\partial y} \frac{\partial}{\partial x''}$$

$$= \frac{1}{\ell''} \frac{\partial}{\partial x''}$$

$$\frac{\partial^2}{\partial y^2} = \frac{1}{\ell''^2} \frac{\partial^2}{\partial x''^2} .$$

The insulation layer temperature equation becomes

$$\frac{k_s''}{\ell''^2} \frac{\partial^2 T_s}{\partial x''^2} + \frac{1}{\ell''^2} \frac{\partial k_s''}{\partial x''} \frac{\partial T_s}{\partial x''} - \rho_s'' \hat{C}_{p_s}'' \frac{\partial T_s}{\partial t} = 0 \quad (4-67)$$

or

$$\frac{\partial^2 T_s}{\partial x''^2} + \alpha_1'' \frac{\partial T_s}{\partial x''} + \alpha_2'' T_s + \alpha_3'' + \alpha_4'' \frac{\partial T_s}{\partial t} = 0 \quad (4-68)$$

where

$$\alpha_1'' = \frac{1}{k_s''} \frac{\partial k_s''}{\partial x''} \quad (4-69)$$

$$\alpha_2'' = 0 \quad (4-70)$$

$$\alpha_3'' = 0 \quad (4-71)$$

$$\alpha_4'' = - \frac{\rho_s'' \hat{C}_{ps}'' \ell''^2}{k_s''} \quad (4-72)$$

#### Boundary Conditions

The transformed boundary conditions are as follows:

Rate of surface removal by oxidation

$$\dot{m}_s = \frac{k P_e C_e \bar{M}_w}{M_{O_2} + \frac{k P_e (H_e - H_w)}{\lambda N_{Le}^{0.6} q_{c,net}}} \quad (4-73)$$

Energy balance at the front surface

$$\begin{aligned} & q_c (1 - H_w/H_e) \left\{ 1 - (1 - \beta) \left[ 0.724 \frac{\hat{H}_e \dot{m}_T}{q_c} - 0.13 \left( \frac{\hat{H}_e \dot{m}_T}{q_c} \right)^2 \right] \right. \\ & \quad \left. - \beta \bar{\eta} \dot{m}_T \frac{\hat{H}_e}{q_c} \right\} + \alpha q_R + \left[ 1 - S(T_{s1} - \bar{T}_1) \right] \dot{m}_s \Delta H_c \\ & = \sigma \epsilon_s T_{s1}^4 - \frac{k_s}{\ell} \frac{\partial T_s}{\partial x} + S(T_{s1} - \bar{T}_1) \dot{m}_s H_c \end{aligned} \quad (4-74)$$

Energy balance at the pyrolysis zone

$$-\left(\frac{k_s}{\ell} \frac{\partial T_s}{\partial x}\right)_{x=1} = \dot{m}_g \Delta H_p - \left(\frac{k'_s}{\ell'} \frac{\partial T_s}{\partial x'}\right)_{x'=0} \quad (4-75)$$

Rate of pyrolysis of uncharred material

$$\dot{m}_g = A' \exp\left(-B'/T_s\right)_{x=1} \quad (4-76)$$

Energy balance at the interface of the uncharred layer and the insulation layer

$$\begin{aligned} -\left(\frac{k'_s}{\ell'} \frac{\partial T_s}{\partial x'}\right)_{x'=1} &= -\left(\frac{k''_s}{\ell''} \frac{\partial T_s}{\partial x''}\right)_{x''=0} \\ &+ \rho_{HS} \hat{C}_{P_{HS}} \ell_{HS} \left(\frac{\partial T_s}{\partial t}\right)_{x'=1} \end{aligned} \quad (4-77)$$

Energy balance at the back surface of the insulation layer

$$\begin{aligned} -\left(\frac{k''_s}{\ell''} \frac{\partial T_s}{\partial x''}\right)_{x''=1} &= \sigma \epsilon''_s T_s^4_{x''=1} - q_B \\ &+ \rho_{HSP} \hat{C}_{P_{HSP}} \ell_{HSP} \left(\frac{\partial T_s}{\partial t}\right)_{x''=1} \end{aligned} \quad (4-78)$$

Specified char porosity at the pyrolysis zone

$$\eta_{x=1} = \eta_0 \quad (4-79)$$

Specified temperature of pyrolysis gas at the pyrolysis interface

$$T_{x=1} = T_{s_{x=1}} \quad (4-80)$$

Specified pressure at the front surface

$$P_x = 0 = P_w \quad (4-81)$$

Specified pressure gradient at the pyrolysis interface

$$\left( \frac{\partial}{\partial x} P^2 \right)_{x=1} = 2\ell R_u \left( \frac{\mu T}{K\bar{M}} \right)_{x=1} \dot{m}_g \quad (4-82)$$

Specified mass flow rate at the pyrolysis interface

$$(\dot{m})_{x=1} = \dot{m}_g \quad (4-83)$$

Specified chemical species mass flow rate at the pyrolysis interface

$$(\rho_i v)_{x=1} = - \left( \frac{x_i}{\eta \bar{M}} \right)_{x=1} M_i \dot{m}_g \quad (4-84)$$

## CHAPTER V

### FINITE DIFFERENCE EQUATIONS

The system of equations derived in Chapter II of this paper includes six partial differential equations with variable coefficients thus it is necessary to solve them numerically. The procedure employed to solve all equations except the total mass conservation equation involves deriving the governing differential equations in finite difference form and solving the resulting sets of algebraic equations by iteration. The total mass conservation equation is solved by numerical integration from the char layer - uncharred layer interface.

Figure 4 shows the locations of the finite-difference stations and the boundary conditions at each boundary. The distances between stations in the char layer, the uncharred layer, and the insulation layer are

$$\left. \begin{aligned} \Delta x &= 1/I - 1 \\ \Delta x' &= 1/J \\ \Delta x'' &= 1/K \end{aligned} \right\} \quad (5-1)$$

The station coordinates are

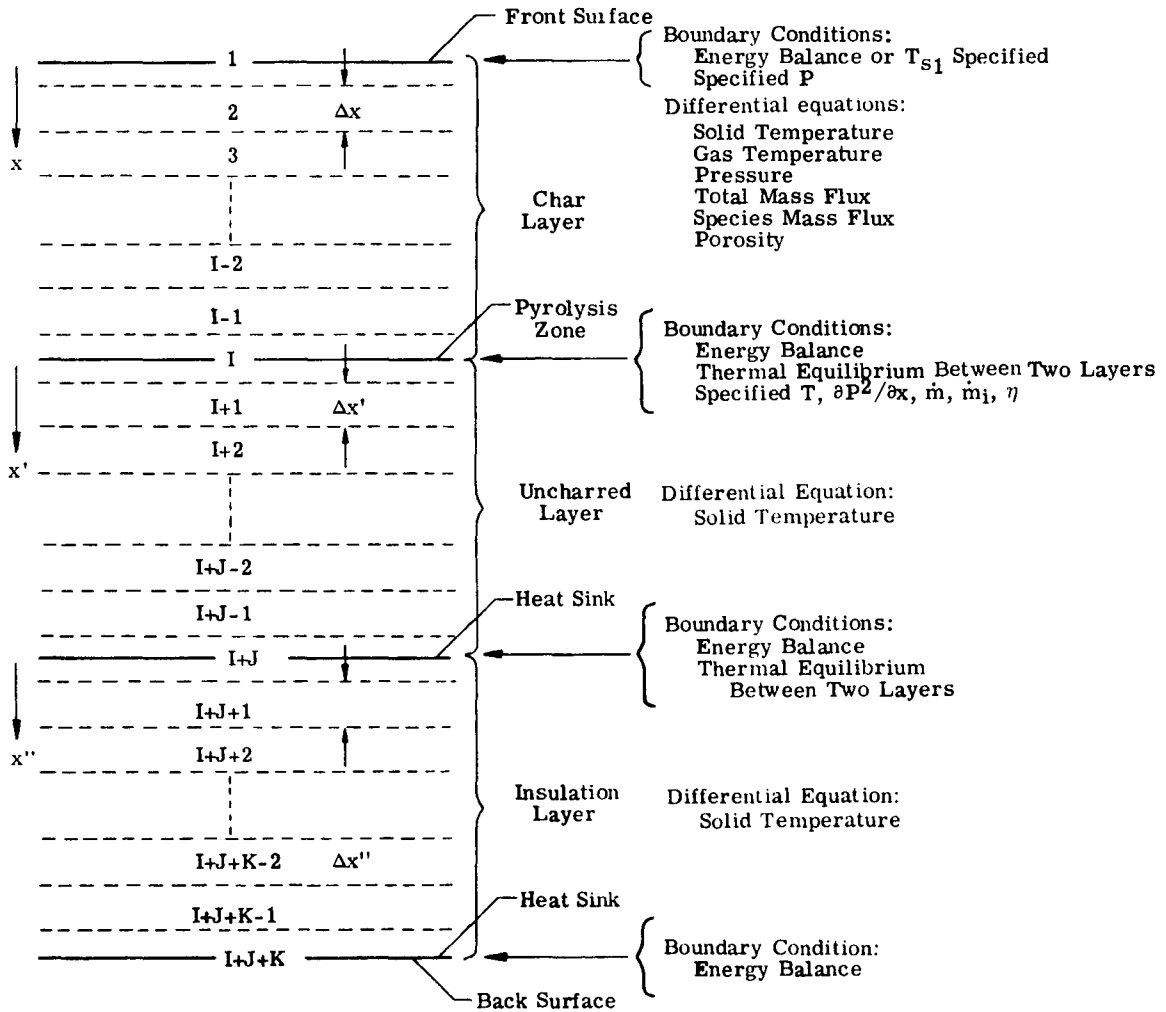


Figure 4.- Location of finite difference stations.



$$x = (N - 1)\Delta x \quad (5-2)$$

for the char layer,

$$x' = (N - 1)\Delta x' \quad (5-3)$$

for the uncharred layer, and

$$x'' = (N - I - J) \Delta x'' \quad (5-4)$$

for the insulation layer.

#### Solid Phase Temperature Equations

The differential equation for the char temperature is

$$\frac{\partial^2 T_s}{\partial x^2} + \alpha_1 \frac{\partial T_s}{\partial x} + \alpha_2 T_s + \alpha_3 + \alpha_4 \frac{\partial T_s}{\partial t} = 0. \quad (5-5)$$

Interior stations of the char layer.— At interior stations the partial derivatives are replaced by central difference approximations. The central difference approximations of the partial derivative are obtained from Taylor series expansions at the station  $N$  evaluated at  $N + 1$  and  $N - 1$ . Thus

$$T_s(N + 1) = T_s(N) + \left( \frac{\partial T_s}{\partial x} \right)_N \Delta x + \left( \frac{\partial^2 T_s}{\partial x^2} \right)_N \frac{\Delta x^2}{2!}$$

$$+ \left( \frac{\partial^3 T_s}{\partial x^3} \right)_N \frac{\Delta x^3}{3!} + \dots \quad (5-6)$$

$$T_s(N-1) = T_s(N) - \left( \frac{\partial T_s}{\partial x} \right)_N \Delta x + \left( \frac{\partial^2 T_s}{\partial x^2} \right)_N \frac{\Delta x^2}{2!} - \left( \frac{\partial^3 T_s}{\partial x^3} \right)_N \frac{\Delta x^3}{3!} + \dots \quad (5-7)$$

Subtracting Eq. 5-7 from Eq. 5-6 gives

$$\left( \frac{\partial T_s}{\partial x} \right)_N = \frac{T_s(N+1) - T_s(N-1)}{2\Delta x} - \left( \frac{\partial^3 T_s}{\partial x^3} \right)_N \frac{\Delta x^2}{12} \quad (5-8)$$

Therefore the equation

$$\left( \frac{\partial T_s}{\partial x} \right)_N = \frac{T_s(N+1) - T_s(N-1)}{2\Delta x} \quad (5-9)$$

is accurate to terms of the order  $\Delta x^2$ . Similarly, adding Eqs. 5-6 and 5-7 gives

$$\left( \frac{\partial^2 T_s}{\partial x^2} \right)_N = \frac{T_s(N+1) - 2T_s(N) + T_s(N-1)}{\Delta x^2} \quad (5-10)$$

which is accurate to terms of the order  $\Delta x^2$ .

Equations 5-9 and 5-10 are used in Eq. 5-5 to obtain

$$\begin{aligned}
& \frac{1}{\Delta x^2} [T_s(N+1) - 2T_s(N) + T_s(N-1)] + \frac{\alpha_1(N)}{2\Delta x} [T_s(N+1) \\
& - T_s(N-1)] + \alpha_2(N) T_s(N) + \alpha_3(N) \\
& + \alpha_4(N) \left( \frac{\partial T_s}{\partial t} \right)_N = 0, \quad (5-11)
\end{aligned}$$

The finite difference approximation of the last term to the left in Eq. 5-11 is obtained from Taylor series expansions at time  $P + \Delta t/2$  evaluated at time  $P$  and  $P + \Delta t$ . Thus

$$\begin{aligned}
\left( \alpha_4 \frac{\partial T_s}{\partial t} \right)^P &= \left( \alpha_4 \frac{\partial T_s}{\partial t} \right)^{P + \Delta t/2} - \frac{\Delta t}{2} \left[ \frac{\partial}{\partial t} \left( \alpha_4 \frac{\partial T_s}{\partial t} \right) \right]^{P + \Delta t/2} \\
&+ \frac{\Delta t^2}{4} \left[ \frac{\partial^2}{\partial t^2} \left( \alpha_4 \frac{\partial T_s}{\partial t} \right) \right]^{P + \Delta t/2} + \dots \quad (5-12)
\end{aligned}$$

$$\begin{aligned}
\left( \alpha_4 \frac{\partial T_s}{\partial t} \right)^{P + \Delta t} &= \left( \alpha_4 \frac{\partial T_s}{\partial t} \right)^{P + \Delta t/2} + \frac{\Delta t}{2} \left[ \frac{\partial}{\partial t} \left( \alpha_4 \frac{\partial T_s}{\partial t} \right) \right]^{P + \Delta t/2} \\
&+ \frac{\Delta t^2}{4} \left[ \frac{\partial^2}{\partial t^2} \left( \alpha_4 \frac{\partial T_s}{\partial t} \right) \right]^{P + \Delta t/2} + \dots ; \quad (5-13)
\end{aligned}$$

Solving these two equations for  $\left( \alpha_4 \frac{\partial T_s}{\partial t} \right)^{P + \Delta t/2}$ ,

$$\left( \alpha_4 \frac{\partial T_s}{\partial t} \right)^{P + \Delta t/2} = \frac{1}{2} \left[ \alpha_4^P \frac{\partial T_s}{\partial t}^P + \alpha_4^{P + \Delta t} \frac{\partial T_s}{\partial t}^{P + \Delta t} \right] \quad (5-14)$$

which is accurate to terms of the order  $\Delta t^2$ . Now

$$\alpha_4^{P + \Delta t/2} = \frac{1}{2} \left( \alpha_4^P + \alpha_4^{P + \Delta t} \right) \quad (5-15)$$

$$\frac{\partial T_s}{\partial t}^{P + \Delta t/2} = \frac{T_s^{P + \Delta t} - T_s^P}{\Delta t} \quad (5-16)$$

and  $\alpha_4^P \frac{\partial T_s}{\partial t}^P$  and  $\alpha_4^{P + \Delta t} \frac{\partial T_s}{\partial t}^{P + \Delta t}$  are obtained from the explicit and implicit formulations of Eq. 5-11, that is

$$\begin{aligned} \left( \alpha_4 \frac{\partial T_s}{\partial t} \right)_N^P &= - \frac{1}{\Delta x^2} [T_s(N+1)^P - 2 T_s(N)^P + T_s(N-1)^P] \\ &\quad - \frac{\alpha_1(N)^P}{2\Delta x} [T_s(N+1)^P - T_s(N-1)^P] - \alpha_2(N)^P T_s(N)^P \\ &\quad - \alpha_3(N)^P \end{aligned} \quad (5-17)$$

$$\begin{aligned} \left( \alpha_4 \frac{\partial T_s}{\partial t} \right)_N^{P + \Delta t} &= - \frac{1}{\Delta x^2} [T_s(N+1)^{P + \Delta t} - 2 T_s(N)^{P + \Delta t} + T_s(N-1)^{P + \Delta t}] \\ &\quad - \frac{\alpha_1(N)^{P + \Delta t}}{2\Delta x} [T_s(N+1)^{P + \Delta t} - T_s(N-1)^{P + \Delta t}] - \alpha_2(N)^{P + \Delta t} T_s(N)^{P + \Delta t} \\ &\quad - \alpha_3(N)^{P + \Delta t} \end{aligned} \quad (5-18)$$

Therefore, the modified implicit finite difference equation for  $T_s$  at interior stations is

$$\begin{aligned}
& [\alpha_4(N)^P + \alpha_4(N)^{P+\Delta t}] \left( \frac{T_s(N)^{P+\Delta t} - T_s(N)^P}{\Delta t} \right) + \frac{1}{\Delta x^2} [T_s(N+1)^P \\
& - 2 T_s(N)^P + T_s(N-1)^P] + \frac{\alpha_1(N)^P}{2\Delta x} [T_s(N+1)^P - T_s(N-1)^P] \\
& + \alpha_2(N)^P T_s(N)^P + \alpha_3(N)^P + \frac{1}{\Delta x^2} [T_s(N+1)^{P+\Delta t} - 2 T_s(N)^{P+\Delta t} \\
& + T_s(N-1)^{P+\Delta t}] + \frac{\alpha_1(N)^{P+\Delta t}}{2\Delta x} [T_s(N+1)^{P+\Delta t} - T_s(N-1)^{P+\Delta t}] \\
& + \alpha_2(N)^{P+\Delta t} T_s(N)^{P+\Delta t} + \alpha_3(N)^{P+\Delta t} = 0 \tag{5-19}
\end{aligned}$$

or

$$\begin{aligned}
& A_s(N) T_s(N-1)^{P+\Delta t} + B_s(N) T_s(N)^{P+\Delta t} + C_s(N) T_s(N+1)^{P+\Delta t} \\
& = D_s(N) \tag{5-20}
\end{aligned}$$

where

$$A_s(N) = 1/\Delta x^2 - \alpha_1(N)^{P+\Delta t}/2\Delta x \tag{5-21}$$

$$B_s(N) = \alpha_2(N)^{P+\Delta t} - 2/\Delta x^2 + \frac{1}{\Delta t} [\alpha_4(N)^P + \alpha_4(N)^{P+\Delta t}] \tag{5-22}$$

$$C_s(N) = 1/\Delta x^2 + \alpha_1(N)^{P+\Delta t}/2\Delta x \tag{5-23}$$

$$\begin{aligned}
D_s(N) = & -\alpha_3(N)^P - \alpha_3(N)^P + \Delta t \left[ \frac{1}{\Delta x^2} - \frac{\alpha_1(N)^P}{2\Delta x} \right] T_s(N-1) \\
& - \{ \alpha_2(N)^P - 2/\Delta x^2 - \frac{1}{\Delta t} [\alpha_4(N)^P + \alpha_4(N)^P + \Delta t] \} T_s(N)^P \\
& - \left[ \frac{1}{\Delta x^2} + \frac{\alpha_1(N)^P}{2\Delta x} \right] T_s(N+1)^P \quad (5-24)
\end{aligned}$$

Interior stations of the uncharred layer.— The modified implicit finite difference equation at interior stations of the uncharred layer is obtained by analogy from Eq. 5-19. The resulting equation is

$$\begin{aligned}
A'_s(N) T_s(N-1)^{P+\Delta t} + B'_s(N) T_s(N)^{P+\Delta t} + C'_s T_s(N+1)^{P+\Delta t} \\
= D'_s(N) \quad (5-25)
\end{aligned}$$

where

$$A'_s(N) = 1/\Delta x'^2 - \frac{\alpha_1(N)^{P+\Delta t}}{2\Delta x'} \quad (5-26)$$

$$B'_s(N) = \alpha_2(N)^{P+\Delta t} - \frac{2}{\Delta x'^2} + \frac{1}{\Delta t} [\alpha_4'(N)^P + \alpha_4'(N)^{P+\Delta t}] \quad (5-27)$$

$$C'_s(N) = 1/\Delta x'^2 + \frac{\alpha_1(N)^{P+\Delta t}}{2\Delta x'} \quad (5-28)$$

$$\begin{aligned}
D'_s(N) = & -\alpha'_3(N)^P - \alpha'_3(N)^P + \Delta t - \left[ \frac{1}{\Delta x'^2} - \frac{\alpha'_1(N)^P}{2\Delta x'} \right] T_s(N-1)^P \\
& - \left\{ \alpha'_2(N)^P - \frac{2}{\Delta x'^2} - \frac{1}{\Delta t} [\alpha'_4(N)^P + \alpha'_4(N)^P + \Delta t] \right\} T_s(N)^P \\
& - \left[ \frac{1}{\Delta x'^2} + \frac{\alpha'_1(N)^P}{2\Delta x'} \right] T_s(N+1)^P
\end{aligned} \tag{5-29}$$

Interior stations of the insulation.— The modified implicit finite difference equation at interior stations of the insulation layer is similarly obtained as

$$\begin{aligned}
A''_s(N) T_s(N-1)^{P+\Delta t} + B''_s(N) T_s(N)^{P+\Delta t} + C''_s(N) T_s(N+1)^{P+\Delta t} \\
= D''_s(N)
\end{aligned} \tag{5-30}$$

where

$$A''_s(N) = 1/\Delta x''^2 - \frac{\alpha''_1(N)^{P+\Delta t}}{2\Delta x''} \tag{5-31}$$

$$B''_s(N) = \alpha''_2(N)^{P+\Delta t} - 2/\Delta x''^2 + \frac{1}{\Delta t} [\alpha''_4(N)^P + \alpha''_4(N)^{P+\Delta t}] \tag{5-32}$$

$$C''_s(N) = 1/\Delta x''^2 + \frac{\alpha''_1(N)^{P+\Delta t}}{2\Delta x''} \tag{5-33}$$

$$D''_s(N) = -\alpha''_3(N)^P - \alpha''_3(N)^{P+\Delta t} - \left[ \frac{1}{\Delta x''^2} - \frac{\alpha''_1(N)^P}{2\Delta x''} \right] T_s(N-1)^P$$

$$\begin{aligned}
& - \{ \alpha_2''(N)^P - \frac{2}{\Delta x''^2} - \frac{1}{\Delta t} [\alpha_4''(N)^P + \alpha_4''(N)^P + \Delta t] \} T_s(N)^P \\
& - \left[ \frac{1}{\Delta x''^2} + \frac{\alpha_1''(N)^P}{2\Delta x''} \right] T_s(N+1)^P.
\end{aligned} \tag{5-34}$$

Boundary stations.— Boundary conditions other than a parameter being specified at a point are employed by combining the governing differential equation and the equation expressing the boundary condition to obtain a differential equation which is valid only at the boundary. The solution of this equation satisfies both the boundary condition and the governing differential equation.

At the front surface (N = 1).— The front surface boundary condition is

$$- \frac{1}{\ell} \left( k_s \frac{\partial T_s}{\partial x} \right)_{N=1} = q_{c,net} - \sigma \epsilon_s T_{s1}^4. \tag{5-35}$$

The second order derivative term in Eq. 5-5 is written as

$$\frac{\partial^2 T_s}{\partial x^2} = \frac{\partial}{\partial x} \left( \frac{\partial T_s}{\partial x} \right). \tag{5-36}$$

The derivative of the temperature gradient is obtained from Taylor series expansions at the station  $N = 1$  evaluated at  $N = 2$ ,  $N = 3$ , and  $N = 4$ . Thus



$$\begin{aligned} \left( \frac{\partial T_s}{\partial x} \right)_{N=2} &= \left( \frac{\partial T_s}{\partial x} \right)_{N=1} + \Delta x \left[ \frac{\partial}{\partial x} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \frac{\Delta x^2}{2} \left[ \frac{\partial^2}{\partial x^2} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} \\ &+ \frac{\Delta x^3}{6} \left[ \frac{\partial^3}{\partial x^3} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \frac{\Delta x^4}{24} \left[ \frac{\partial^4}{\partial x^4} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \dots \quad (5-37) \end{aligned}$$

$$\begin{aligned} \left( \frac{\partial T_s}{\partial x} \right)_{N=3} &= \left( \frac{\partial T_s}{\partial x} \right)_{N=1} + 2\Delta x \left[ \frac{\partial}{\partial x} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + 2\Delta x^2 \left[ \frac{\partial^2}{\partial x^2} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} \\ &+ \frac{4\Delta x^3}{3} \left[ \frac{\partial^3}{\partial x^3} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \frac{2\Delta x^4}{3} \left[ \frac{\partial^4}{\partial x^4} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \dots \quad (5-38) \end{aligned}$$

$$\begin{aligned} \left( \frac{\partial T_s}{\partial x} \right)_{N=4} &= \left( \frac{\partial T_s}{\partial x} \right)_{N=1} + 3\Delta x \left[ \frac{\partial}{\partial x} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \frac{9\Delta x^2}{2} \left[ \frac{\partial^2}{\partial x^2} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} \\ &+ \frac{9}{2} \Delta x^3 \left[ \frac{\partial^3}{\partial x^3} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \frac{27}{8} \Delta x^4 \left[ \frac{\partial^4}{\partial x^4} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} + \dots \quad (5-39) \end{aligned}$$

Solving for  $\left[ \frac{\partial}{\partial x} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1}$

$$\begin{aligned} \left[ \frac{\partial}{\partial x} \left( \frac{\partial T_s}{\partial x} \right) \right]_{N=1} &= \frac{1}{6\Delta x} \left[ -11 \left( \frac{\partial T_s}{\partial x} \right)_{N=1} + 18 \left( \frac{\partial T_s}{\partial x} \right)_{N=2} \right. \\ &\quad \left. - 9 \left( \frac{\partial T_s}{\partial x} \right)_{N=3} + 2 \left( \frac{\partial T_s}{\partial x} \right)_{N=4} \right] \quad (5-40) \end{aligned}$$

which is accurate to terms of the order  $\Delta x^3$ . Therefore,

$$\left( \frac{\partial^2 T_s}{\partial x^2} \right)_{N=1} = \frac{1}{6\Delta x} \left[ -11 \left( \frac{\partial T_s}{\partial x} \right)_{N=1} + 18 \left( \frac{\partial T_s}{\partial x} \right)_{N=2} - 9 \left( \frac{\partial T_s}{\partial x} \right)_{N=3} + 2 \left( \frac{\partial T_s}{\partial x} \right)_{N=4} \right] \quad (5-41)$$

Combining Eq. 5-41 with Eq. 5-5 written for station  $N = 1$  gives

$$\begin{aligned} [\alpha_1(N) - \frac{11}{6\Delta x}] \left( \frac{\partial T_s}{\partial x} \right)_{N=1} + \frac{3}{\Delta x} \left( \frac{\partial T_s}{\partial x} \right)_{N=2} - \frac{3}{2\Delta x} \left( \frac{\partial T_s}{\partial x} \right)_{N=3} \\ + \frac{1}{3\Delta x} \left( \frac{\partial T_s}{\partial x} \right)_{N=4} + \alpha_2(1) T_s(1) + \alpha_3(1) \\ + \alpha_4(1) \left( \frac{\partial T_s}{\partial t} \right)_{N=1} = 0 \end{aligned} \quad (5-42)$$

The temperature gradient at station  $N = 1$  is given by Eq. 5-35. The temperature gradients of neighboring stations are approximated by central difference expressions. The resulting finite difference equation is

$$\begin{aligned} \{ [\alpha_1(1) - \frac{11}{6\Delta x}] \frac{\ell}{k_s(1)} \sigma \epsilon_s T_s(1)^3 - \frac{3}{2\Delta x^2} + \alpha_2(1) \} T_s(1) \\ + \frac{3}{4\Delta x^2} T_s(2) + \left( \frac{3}{2\Delta x^2} - \frac{1}{6\Delta x^2} \right) T_s(3) - \frac{3}{4\Delta x^2} T_s(4) \\ + \frac{1}{6\Delta x^2} T_s(5) + \alpha_3(1) - \frac{q_{c,net} \ell}{k_s(1)} [\alpha_1(1) - \frac{11}{6\Delta x}] \\ + \alpha_4(1) \left( \frac{\partial T_s}{\partial t} \right)_{N=1} = 0 \end{aligned} \quad (5-43)$$

Following the procedure used to obtain the modified implicit finite difference equation for interior stations, the analogous equation for the station at the front surface becomes

$$\begin{aligned}
& \{ [\alpha_1(1)^{P+\Delta t} - \frac{11}{6\Delta x}] \frac{\ell^{P+\Delta t}}{k_s(1)^{P+\Delta t}} \sigma \epsilon_s [T_s(1)^{P+\Delta t}]^3 - \frac{3}{2\Delta x^2} \\
& + \alpha_2(1)^{P+\Delta t} + \frac{1}{\Delta t} [\alpha_4(1)^P + \alpha_4(1)^{P+\Delta t}] \} T_s(1)^{P+\Delta t} \\
& + 3/4\Delta x^2 T_s(2)^{P+\Delta t} + \left( \frac{3}{2\Delta x^2} - \frac{1}{6\Delta x^2} \right) T_s(3)^{P+\Delta t} - \frac{3}{4\Delta x^2} T_s(4)^{P+\Delta t} \\
& + \frac{1}{6\Delta x^2} T_s(5)^{P+\Delta t} = -\alpha_3(1)^P - \alpha_3(1)^{P+\Delta t} + [\alpha_1(1)^{P+\Delta t} \\
& - \frac{11}{6\Delta x}] q_{c,net}^{P+\Delta t} \frac{\ell^{P+\Delta t}}{k_s(1)^{P+\Delta t}} + [\alpha_1(1)^P - \frac{11}{6\Delta x}] q_{c,net}^P \frac{\ell^P}{k_s(1)^P} \\
& - \{ [\alpha_1(1)^P - \frac{11}{6\Delta x}] \frac{\ell^P}{k_s(1)^P} \sigma \epsilon_s [T_s(1)^P]^3 - \frac{3}{2\Delta x^2} \\
& + \alpha_2(1)^P - \frac{1}{\Delta t} [\alpha_4(1)^P + \alpha_4(1)^{P+\Delta t}] \} T_s(1)^P \\
& - \frac{3}{4\Delta x^2} T_s(2)^P - \left( \frac{3}{2\Delta x^2} - \frac{1}{6\Delta x^2} \right) T_s(3)^P + 3/4\Delta x^2 T_s(4)^P \\
& - \frac{1}{6\Delta x^2} T_s(5)^P
\end{aligned} \tag{5-44}$$

or

$$\begin{aligned}
& B1_s T_s(1)^{P + \Delta t} + C1_s T_s(2)^{P + \Delta t} + G1_s T_s(3)^{P + \Delta t} \\
& + H1_s T_s(4)^{P + \Delta t} + I1_s T_s(5)^{P + \Delta t} = D1_s
\end{aligned} \tag{5-45}$$

where

$$\begin{aligned}
B1_s = & [\alpha_1(1)^{P + \Delta t} - \frac{11}{6\Delta x}] \frac{\ell^{P + \Delta t}}{k_s(1)^{P + \Delta t}} \sigma \epsilon_s [T_s(1)^{P + \Delta t}]^3 \\
& - \frac{3}{2\Delta x^2} + \alpha_2(1)^{P + \Delta t} + \frac{1}{\Delta t} [\alpha_4(1)^P + \alpha_4(1)^{P + \Delta t}]
\end{aligned} \tag{5-46}$$

$$C1_s = 3/8\Delta x^2 \tag{5-47}$$

$$G1_s = \frac{3}{4\Delta x^2} - \frac{1}{12\Delta x^2} \tag{5-48}$$

$$H1_s = -\frac{3}{8\Delta x^2} \tag{5-49}$$

$$I1_s = \frac{1}{12\Delta x^2} \tag{5-50}$$

$$\begin{aligned}
D1_s = & -\alpha_3(1)^P - \alpha_3(1)^{P + \Delta t} + [\alpha_1(1)^{P + \Delta t} - \frac{11}{6\Delta x}] q_{c,net} \frac{\ell^{P + \Delta t}}{k_s(1)^{P + \Delta t}} \\
& + [\alpha_1(1)^P - \frac{11}{6\Delta x}] q_{c,net} \frac{\ell^P}{k_s(1)^P} - \{[\alpha_1(1)^P \\
& - \frac{11}{6\Delta x}] \frac{\ell^P}{k_s(1)^P} \sigma \epsilon_s [T_s(1)^P]^3 - \frac{3}{2\Delta x^2} + \alpha_2(1)^P
\end{aligned}$$

$$\begin{aligned}
& - \frac{1}{\Delta t} [\alpha_4(1)^P + \alpha_4(1)^P + \Delta t] \} T_s(1)^P - \frac{3}{4\Delta x^2} T_s(2)^P \\
& - \left( \frac{3}{2\Delta x^2} - \frac{1}{6\Delta x^2} \right) T_s(3)^P + \frac{3}{4\Delta x^2} T_s(4)^P \\
& - \frac{1}{6\Delta x^2} T_s(5)^P, \tag{5-51}
\end{aligned}$$

At the pyrolysis zone (N = I).— The boundary condition at the pyrolysis zone is

$$- \frac{1}{\ell} \left( k_s \frac{\partial T_s}{\partial x} \right)_{N=I} = \dot{m}_g \Delta H_p - \frac{1}{\ell'} \left( k'_s \frac{\partial T_s}{\partial x'} \right)_{N=I}, \tag{5-52}$$

The second order derivative in the governing equation for char layer temperature is approximated by a four-point backward difference expression analogous to Eq. 5-41. Thus

$$\begin{aligned}
\left( \frac{\partial^2 T_s}{\partial x^2} \right)_{N=I} &= \frac{1}{6\Delta x} \left[ 11 \left( \frac{\partial T_s}{\partial x} \right)_{N=I} - 18 \left( \frac{\partial T_s}{\partial x} \right)_{N=I-1} \right. \\
&\quad \left. + 9 \left( \frac{\partial T_s}{\partial x} \right)_{N=I-2} - 2 \left( \frac{\partial T_s}{\partial x} \right)_{N=I-3} \right]. \tag{5-53}
\end{aligned}$$

Using this equation in the governing equation for char layer temperature and solving for the char layer temperature gradient at the pyrolysis zone gives

$$\begin{aligned}
\left(\frac{\partial T_s}{\partial x}\right)_{N=1} &= \frac{6}{11} \left[ 3 \left(\frac{\partial T_s}{\partial x}\right)_{N=I-1} - \frac{3}{2} \left(\frac{\partial T_s}{\partial x}\right)_{N=I-2} \right. \\
&\quad + \frac{1}{3} \left(\frac{\partial T_s}{\partial x}\right)_{N=1-3} - \alpha_1(I) \Delta x \left(\frac{\partial T_s}{\partial x}\right)_{N=I} \\
&\quad - \alpha_2(I) \Delta x T_s(I) - \alpha_3(I) \Delta x \\
&\quad \left. - \alpha_4(I) \Delta x \frac{\partial T_s}{\partial t} \right]_{N=I} . \tag{5-54}
\end{aligned}$$

The analogous expression for the uncharred layer temperature gradient is

$$\begin{aligned}
\left(\frac{\partial T_s}{\partial x'}\right)_{N=I} &= \frac{6}{11} \left[ 3 \left(\frac{\partial T_s}{\partial x}\right)_{N=I+1} - \frac{3}{2} \left(\frac{\partial T_s}{\partial x}\right)_{N=I+2} + \frac{1}{3} \left(\frac{\partial T_s}{\partial x}\right)_{N=I+3} \right. \\
&\quad + \alpha'_1(I) \Delta x' \left(\frac{\partial T_s}{\partial x}\right)_{N=I} + \alpha'_2(I) \Delta x' T_s(I) \\
&\quad \left. + \alpha'_3(I) \Delta x' + \alpha'_4(I) \Delta x' \left(\frac{\partial T_s}{\partial t}\right)_{N=I} \right] , \tag{5-55}
\end{aligned}$$

Combining Eqs. 5-52, 5-54, and 5-55 gives

$$\begin{aligned}
\left(\frac{\partial T_s}{\partial t}\right)_{N=I} &= \frac{1}{\frac{\Delta x k_s(I) \alpha_4(I)}{\ell} + \frac{\Delta x' k'_s(I) \alpha'_4(I)}{\ell'}} \left\{ \frac{k_s(I)}{\ell} \left[ 3 \left(\frac{\partial T_s}{\partial x}\right)_{N=I-1} \right. \right. \\
&\quad \left. - \frac{3}{2} \left(\frac{\partial T_s}{\partial x}\right)_{N=I-2} + \frac{1}{3} \left(\frac{\partial T_s}{\partial x}\right)_{N=I-3} - \alpha_1(I) \Delta x \left(\frac{\partial T_s}{\partial x}\right)_{N=I} - \alpha_2(I) \Delta x T_s(I) \right. \\
&\quad \left. \left. + \alpha'_1(I) \Delta x' \left(\frac{\partial T_s}{\partial x}\right)_{N=I} + \alpha'_2(I) \Delta x' T_s(I) + \alpha'_3(I) \Delta x' + \alpha'_4(I) \Delta x' \left(\frac{\partial T_s}{\partial t}\right)_{N=I} \right] \right\} ,
\end{aligned}$$

$$\begin{aligned}
& - \alpha_3(I) \Delta x \left] + \frac{11}{6} \dot{m}_g \Delta H_p - \frac{k'_s(I)}{\ell'} \left[ 3 \left( \frac{\partial T_s}{\partial x} \right)_{N=I+1} - \frac{3}{2} \left( \frac{\partial T_s}{\partial x} \right)_{N=I+2} \right. \right. \\
& + \frac{1}{3} \left( \frac{\partial T_s}{\partial x} \right)_{N=I+3} + \alpha'_1(I) \Delta x' \left( \frac{\partial T_s}{\partial x'} \right)_I + \alpha'_2(I) \Delta x' T_s(I) \\
& \left. \left. + \alpha'_3(I) \Delta x' \right] \right\} \quad (5-56)
\end{aligned}$$

which is valid at the pyrolysis zone.

Approximating the temperature gradient of the char layer and the uncharred layer by four-point backward difference and forward difference expressions, respectively, and using central difference approximations for the temperature gradients at interior stations gives

$$\begin{aligned}
\left( \frac{\partial T_s}{\partial t} \right)_{N=I} &= \frac{1}{\frac{k_s(I) \alpha_4(I) \Delta x}{\ell} + \frac{k'_s(I) \alpha'_4(I) \Delta x'}{\ell'}} \left\{ \frac{k_s(I)}{\ell} \left[ - \frac{1}{6 \Delta x} T_s(I-4) \right. \right. \\
& + \left( \frac{3}{4 \Delta x} + \frac{\alpha_1(I)}{3} \right) T_s(I-3) - \left( \frac{4}{3 \Delta x} + \frac{3 \alpha_1(I)}{2} \right) T_s(I-2) \\
& - \left. \left( \frac{3}{4 \Delta x} - 3 \alpha_1(I) \right) T_s(I-1) \right] + \left[ \frac{k_s(I)}{\ell} \left( \frac{3}{2 \Delta x} - \frac{11}{6} \alpha_1(I) \right. \right. \\
& - \alpha_2(I) \Delta x \left. \right) + \frac{k'_s(I)}{\ell'} \left( \frac{3}{2 \Delta x} + \frac{11}{6} \alpha'_1(I) - \alpha'_2(I) \Delta x' \right) \left. \right] T_s(I) \\
& + \frac{11}{6} \dot{m}_g \Delta H_p - \frac{k_s(I) \alpha_3(I) \Delta x}{\ell} - \frac{k'_s(I) \alpha'_3(I) \Delta x'}{\ell} \\
& - \frac{k'_s(I)}{\ell'} \left[ \left( \frac{3}{4 \Delta x'} + 3 \alpha'_1(I) \right) T_s(I+1) + \left( \frac{4}{3 \Delta x'} - \frac{3 \alpha_1(I)}{2} \right) T_s(I+2) \right. \\
& - \left. \left( \frac{3}{4 \Delta x'} - \frac{\alpha_1(I)}{3} \right) T_s(I+3) + \frac{1}{6 \Delta x'} T_s(I+4) \right] \left. \right\} \quad (5-57)
\end{aligned}$$

The modified implicit finite difference equation results from taking an average of Eq. 5-57 written in explicit form and in implicit form.

The result is

$$\begin{aligned}
 & ZI_s T_s(I-4)^{P+\Delta t} + YI_s T_s(I-3)^{P+\Delta t} + XI_s T_s(I-2)^{P+\Delta t} \\
 & + AI_s T_s(I-1)^{P+\Delta t} + BI_s T_s(I)^{P+\Delta t} \\
 & + CI_s T_s(I+1)^{P+\Delta t} + EI_s T_s(I+2)^{P+\Delta t} \\
 & + FI_s T_s(I+3)^{P+\Delta t} + GI_s T_s(I+4)^{P+\Delta t} \\
 & = DI_s
 \end{aligned} \tag{5-58}$$

where

$$\begin{aligned}
 & -k_s(I)^{P+\Delta t}/(12 \Delta x \ell^{P+\Delta t}) \\
 ZI_s = & \frac{k_s(I)^{P+\Delta t} \alpha_4(I)^{P+\Delta t} \Delta x}{\ell^{P+\Delta t}} + \frac{k'_s(I)^{P+\Delta t} \alpha'_4(I)^{P+\Delta t} \Delta x'}{\ell'^{P+\Delta t}}
 \end{aligned} \tag{5-59}$$

$$\begin{aligned}
 & k_s(I)^{P+\Delta t} \left[ \frac{3}{4\Delta x} + \frac{\alpha_1(x)^{P+\Delta t}}{3} \right] / \ell^{P+\Delta t} \\
 YI_s = & \frac{1}{2} \left[ \frac{k_s(I)^{P+\Delta t} \alpha_4(I)^{P+\Delta t} \Delta x}{\ell^{P+\Delta t}} + \frac{k'_s(I)^{P+\Delta t} \alpha'_4(I)^{P+\Delta t} \Delta x'}{\ell'^{P+\Delta t}} \right]
 \end{aligned} \tag{5-60}$$



$$\begin{aligned}
& -k_s(I)^{P+\Delta t} \left[ \frac{4}{3\Delta x} + \frac{3\alpha_1(x)}{2} \right] / \ell^{P+\Delta t} \\
\text{XI}_s = & \frac{1}{2} \left[ \frac{k_s(I)^{P+\Delta t} \alpha_4(I)^{P+\Delta t} \Delta x}{\ell^{P+\Delta t}} + \frac{k'_s(I)^{P+\Delta t} \alpha'_4(I)^{P+\Delta t} \Delta x'}{\ell', P+\Delta t} \right] \quad (5-61)
\end{aligned}$$

$$\begin{aligned}
& -k_s(I)^{P+\Delta t} \left[ \frac{3}{4\Delta x} - 3\alpha_1(I)^{P+\Delta t} \right] / \ell^{P+\Delta t} \\
\text{AI}_s = & \frac{1}{2} \left[ \frac{k_s(I)^{P+\Delta t} \alpha_4(I)^{P+\Delta t} \Delta x}{\ell^{P+\Delta t}} + \frac{k'_s(I)^{P+\Delta t} \alpha'_4(I)^{P+\Delta t} \Delta x'}{\ell', P+\Delta t} \right] \quad (5-62)
\end{aligned}$$

$$\begin{aligned}
\text{BI}_s = & -\frac{1}{\Delta t} + \frac{1}{2} \left[ \frac{k_s(I)^{P+\Delta t} \alpha_4(I)^{P+\Delta t} \Delta x}{\ell^{P+\Delta t}} + \frac{k'_s(I)^{P+\Delta t} \alpha'_4(I)^{P+\Delta t} \Delta x'}{\ell', P+\Delta t} \right] \\
& \left\{ \frac{k_s(I)^{P+\Delta t}}{\ell^{P+\Delta t}} \left[ \frac{3}{2\Delta x} - \frac{11}{6} \alpha_1(I)^{P+\Delta t} - \alpha_2(I)^{P+\Delta t} \Delta x \right] \right. \\
& \left. + \frac{k'_s(I)^{P+\Delta t}}{\ell', P+\Delta t} \left[ \frac{3}{2\Delta x'} + \frac{11}{6} \alpha'_1(I)^{P+\Delta t} - \alpha'_2(I)^{P+\Delta t} \Delta x' \right] \right\} \quad (5-63)
\end{aligned}$$

$$\begin{aligned}
& -k'_s(I)^{P+\Delta t} \left[ \frac{3}{4\Delta x'} + 3\alpha'_1(I)^{P+\Delta t} \right] / \ell', P+\Delta t \\
\text{CI}_s = & \frac{1}{2} \left[ \frac{k_s(I)^{P+\Delta t} \alpha_4(I)^{P+\Delta t} \Delta x}{\ell^{P+\Delta t}} + \frac{k'_s(I)^{P+\Delta t} \alpha'_4(I)^{P+\Delta t} \Delta x'}{\ell', P+\Delta t} \right] \quad (5-64)
\end{aligned}$$

$$\begin{aligned}
& -k'_s(I)^{P+\Delta t} \left[ \frac{4}{3\Delta x'} + 3\alpha'_1(I)^{P+\Delta t} \right] / \ell', P+\Delta t \\
\text{EI}_s = & \frac{1}{2} \left[ \frac{k_s(I)^{P+\Delta t} \alpha_4(I)^{P+\Delta t} \Delta x}{\ell^{P+\Delta t}} + \frac{k'_s(I)^{P+\Delta t} \alpha'_4(I)^{P+\Delta t} \Delta x'}{\ell', P+\Delta t} \right] \quad (5-65)
\end{aligned}$$

$$FI_s = \frac{k'_s(I)^P + \Delta t \left[ \frac{3}{4\Delta x'} - \frac{1}{3} \alpha'_1(I)^P + \Delta t \right] / \ell,^P + \Delta t}{2 \left[ \frac{k_s(I)^P + \Delta t \alpha_4(I)^P + \Delta t \Delta x}{\ell^P + \Delta t} + \frac{k'_s(I)^P + \Delta t \alpha'_4(I)^P + \Delta t \Delta x'}{\ell',^P + \Delta t} \right]} \quad (5-66)$$

$$GI_s = \frac{-k'_s(I)^P + \Delta t / (12 \Delta x' \ell',^P + \Delta t)}{2 \left[ \frac{k_s(I)^P + \Delta t \alpha_4(I)^P + \Delta t \Delta x}{\ell^P + \Delta t} + \frac{k'_s(I)^P + \Delta t \alpha'_4(I)^P + \Delta t \Delta x'}{\ell',^P + \Delta t} \right]} \quad (5-67)$$

$$DI_s = \frac{1}{2 \left[ \frac{k_s(I)^P + \Delta t \alpha_4(I)^P + \Delta t \Delta x}{\ell^P + \Delta t} + \frac{k'_s(I)^P + \Delta t \alpha'_4(I)^P + \Delta t \Delta x'}{\ell',^P + \Delta t} \right]}$$

$$\left[ \frac{k_s(I)^P + \Delta t \alpha_3(I)^P + \Delta t \Delta x}{\ell^P + \Delta t} + \frac{k'_s(I)^P + \Delta t \alpha'_3(I)^P + \Delta t \Delta x'}{\ell',^P + \Delta t} - \frac{11}{6} \dot{m}_g^P + \Delta t \Delta H_p \right]$$

$$+ \frac{1}{2 \left[ \frac{k_s(I)^P \alpha_4(I)^P \Delta x}{\ell^P} + \frac{k'_s(I)^P \alpha'_4(I)^P \Delta x'}{\ell',^P} \right]} \left[ \frac{k_s(I)^P \alpha_3(I)^P \Delta x}{\ell^P} + \frac{k'_s(I)^P \alpha'_3(I)^P \Delta x'}{\ell',^P} - \frac{11}{6} \dot{m}_g^P \Delta H_p \right]$$

$$- \frac{k_s(I)^P / \ell^P}{2 \left[ \frac{k_s(I)^P \alpha_4(I)^P \Delta x}{\ell^P} + \frac{k'_s(I)^P \alpha'_4(I)^P \Delta x'}{\ell',^P} \right]} \left\{ - \frac{1}{6\Delta x} T_s(I-4)^P \right.$$

$$\begin{aligned}
& + \left[ \frac{3}{4\Delta x} + \frac{\alpha_1(I)^P}{3} \right] T_s(I-3)^P - \left[ \frac{4}{3\Delta x} + \frac{3}{2} \alpha_1(I)^P \right] T_s(I-2)^P \\
& - \left[ \frac{3}{4\Delta x} - 3\alpha_1(I)^P \right] T_s(I-1)^P \Big\} \\
& - \left[ \frac{1}{2 \left[ \frac{k_s(I)^P \alpha_4(I)^P \Delta x}{\ell^P} + \frac{k'_s(I)^P \alpha'_4(I)^P \Delta x'}{\ell'^P} \right]} \right] \left\{ \frac{k_s(I)^P}{\ell^P} \left[ \frac{3}{2\Delta x} \right. \right. \\
& - \frac{11}{6} \alpha_1(I)^P - \alpha_2(I)^P \Delta x \Big] + \frac{k'_s(I)^P}{\ell'^P} \left[ \frac{3}{2\Delta x'} + \frac{11}{6} \alpha'_1(I)^P \right. \\
& \left. \left. - \alpha'_2(I)^P \Delta x' \right] \right\} + \frac{1}{\Delta t} \Big] T_s(I)^P \\
& + \frac{k'_s(I)^P / \ell'^P}{2 \left[ \frac{k_s(I)^P \alpha_4(I)^P \Delta x}{\ell^P} + \frac{k'_s(I)^P \alpha'_4(I)^P \Delta x'}{\ell'^P} \right]} \left\{ \left[ \frac{3}{4\Delta x'} \right. \right. \\
& + 3\alpha'_1(I)^P \Big] T_s(I+1)^P + \left[ \frac{4}{3\Delta x'} - \frac{3}{2} \alpha'_1(I)^P \right] T_s(I+2)^P \\
& \left. - \left[ \frac{3}{4\Delta x'} - \frac{1}{3} \alpha'_1(I)^P \right] T_s(I+3)^P + \frac{1}{6\Delta x'} T_s(I+4)^P \right\} \quad (5-68)
\end{aligned}$$

At the uncharred material - insulation interface (N = I + J).-

The boundary condition at the interface of the uncharred material and the insulation is

$$\begin{aligned}
-\frac{1}{\ell'} \left( k'_s \frac{\partial T_s}{\partial x'} \right)_{N=I+J} - \frac{1}{\ell''} \left( k''_s \frac{\partial T_s}{\partial x''} \right)_{N=I+J} \\
+ \rho_{HS} \hat{C}_{P_{HS}} \ell_{HS} \left( \frac{\partial T_s}{\partial t} \right)_{N=I+J} = 0
\end{aligned} \quad (5-69)$$

This equation is combined with the uncharred material temperature equation and the insulation temperature equation following the procedure used for the pyrolysis zone equations. The resulting modified implicit finite difference equation is

$$\begin{aligned}
& ZP_s T_s (I+J-4)^{P+\Delta t} + YP_s T_s (I+J-3)^{P+\Delta t} \\
& + XP_s T_s (I+J-2)^{P+\Delta t} + AP_s T_s (I+J-1)^{P+\Delta t} \\
& + BP_s T_s (I+J)^{P+\Delta t} + CP_s T_s (I+J+1)^{P+\Delta t} \\
& + EP_s T_s (I+J+2)^{P+\Delta t} + FP_s T_s (I+J+3)^{P+\Delta t} \\
& + GP_s T_s (I+J+4)^{P+\Delta t} = DP_s
\end{aligned} \quad (5-70)$$

where

$$ZP_s = \left[ \frac{k'_s (I+J)^{P+\Delta t} / (12 \Delta' \ell'^{P+\Delta t})}{\ell'^{P+\Delta t}} + \frac{k''_s (I+J)^{P+\Delta t} \alpha''_4 (I+J)^{P+\Delta t} \Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS} \hat{C}_{P_{HS}} \ell_{HS} \right] \quad (5-71)$$

$$Y P_s = \frac{k'_s(I+J)^{P+\Delta t}/\ell, P+\Delta t \left[ \frac{3}{4\Delta x'} + \alpha'_1(I+J)^{P+\Delta t}/3 \right]}{2 \left[ \frac{k'_s(I+J)^{P+\Delta t} \alpha'_4(I+J)^{P+\Delta t} \Delta x'}{\ell, P+\Delta t} + \frac{k''_s(I+J)^{P+\Delta t} \alpha''_4(I+J)^{P+\Delta t} \Delta x''}{\ell'', P+\Delta t} - \rho_{HS} \hat{C}_{P_{HS}}^{\ell_{HS}} \right]} \quad (5-72)$$

$$X P_s = \frac{-k'_s(I+J)^{P+\Delta t}/\ell, P+\Delta t \left[ \frac{4}{3\Delta x'} + \frac{3}{2} \alpha'_1(I+J)^{P+\Delta t} \right]}{2 \left[ \frac{k'_s(I+J)^{P+\Delta t} \alpha'_4(I+J)^{P+\Delta t} \Delta x'}{\ell, P+\Delta t} + \frac{k''_s(I+J)^{P+\Delta t} \alpha''_4(I+J)^{P+\Delta t} \Delta x''}{\ell'', P+\Delta t} - \rho_{HS} \hat{C}_{P_{HS}}^{\ell_{HS}} \right]} \quad (5-73)$$

$$A P_s = \frac{-k'_s(I+J)^{P+\Delta t}/\ell, P+\Delta t \left[ \frac{3}{4\Delta x'} - 3\alpha'_1(I+J)^{P+\Delta t} \right]}{2 \left[ \frac{k'_s(I+J)^{P+\Delta t} \alpha'_4(I+J)^{P+\Delta t} \Delta x'}{\ell, P+\Delta t} + \frac{k''_s(I+J)^{P+\Delta t} \alpha''_4(I+J)^{P+\Delta t} \Delta x''}{\ell'', P+\Delta t} - \rho_{HS} \hat{C}_{P_{HS}}^{\ell_{HS}} \right]} \quad (5-74)$$

$$B P_s = \frac{1}{2 \left[ \frac{k'_s(I+J)^{P+\Delta t} \alpha'_4(I+J)^{P+\Delta t} \Delta x'}{\ell, P+\Delta t} + \frac{k''_s(I+J)^{P+\Delta t} \alpha''_4(I+J)^{P+\Delta t} \Delta x''}{\ell'', P+\Delta t} - \rho_{HS} \hat{C}_{P_{HS}}^{\ell_{HS}} \right]}$$

$$\left\{ \frac{k'_s(I+J)^{P+\Delta t}}{\ell, P+\Delta t} \left[ \frac{3}{2\Delta x'} - \frac{11}{6} \alpha'_1(I+J)^{P+\Delta t} - \alpha'_2(I+J)^{P+\Delta t} \Delta x' \right] + \frac{k''_s(I+J)^{P+\Delta t}}{\ell'', P+\Delta t} \left[ \frac{3}{2\Delta x''} + \frac{11}{6} \alpha''_1(I+J)^{P+\Delta t} - \alpha''_2(I+J)^{P+\Delta t} \Delta x'' \right] \right\} - \frac{1}{\Delta t} \quad (5-75)$$

$$CP_s = \frac{-k_s''(I+J)^{P+\Delta t}/\ell''^{P+\Delta t} \left[ \frac{3}{4\Delta x''} + 3\alpha_1''(I+J)^{P+\Delta t} \right]}{2 \left[ \frac{k_s'(I+J)^{P+\Delta t} \alpha_4'(I+J)^{P+\Delta t} \Delta x'}{\ell'^{P+\Delta t}} + \frac{k_s''(I+J)^{P+\Delta t} \alpha_4''(I+J)^{P+\Delta t} \Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS} \hat{C}_{P_{HS}} \ell_{HS} \right]} \quad (5-76)$$

$$EP_s = \frac{-k_s''(I+J)^{P+\Delta t}/\ell''^{P+\Delta t} \left[ \frac{4}{3\Delta x''} - \frac{3}{2} \alpha_1''(I+J)^{P+\Delta t} \right]}{2 \left[ \frac{k_s'(I+J)^{P+\Delta t} \alpha_4'(I+J)^{P+\Delta t} \Delta x'}{\ell'^{P+\Delta t}} + \frac{k_s''(I+J)^{P+\Delta t} \alpha_4''(I+J)^{P+\Delta t} \Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS} \hat{C}_{P_{HS}} \ell_{HS} \right]} \quad (5-77)$$

$$FP_s = \frac{k_s''(I+J)^{P+\Delta t}/\ell''^{P+\Delta t} \left[ \frac{3}{4\Delta x''} - \frac{1}{3} \alpha_1''(I+J)^{P+\Delta t} \right]}{2 \left[ \frac{k_s'(I+J)^{P+\Delta t} \alpha_4'(I+J)^{P+\Delta t} \Delta x'}{\ell'^{P+\Delta t}} + \frac{k_s''(I+J)^{P+\Delta t} \alpha_4''(I+J)^{P+\Delta t} \Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS} \hat{C}_{P_{HS}} \ell_{HS} \right]} \quad (5-78)$$

$$GP_s = \frac{-k_s''(I+J)^{P+\Delta t}/(12 \Delta x'' \ell''^{P+\Delta t})}{2 \left[ \frac{k_s'(I+J)^{P+\Delta t} \alpha_4'(I+J)^{P+\Delta t} \Delta x'}{\ell'^{P+\Delta t}} + \frac{k_s''(I+J)^{P+\Delta t} \alpha_4''(I+J)^{P+\Delta t} \Delta x''}{\ell''^{P+\Delta t}} - \rho_{HE} \hat{C}_{P_{HS}} \ell_{HS} \right]} \quad (5-79)$$

$$DP_s = \frac{\left[ \frac{k_s'(I+J)^{P+\Delta t} \alpha_3'(I+J)^{P+\Delta t} \Delta x'}{\ell'^{P+\Delta t}} + \frac{k_s''(I+J)^{P+\Delta t} \alpha_3''(I+J)^{P+\Delta t} \Delta x''}{\ell''^{P+\Delta t}} \right]}{2 \left[ \frac{k_s'(I+J)^{P+\Delta t} \alpha_4'(I+J)^{P+\Delta t} \Delta x'}{\ell'^{P+\Delta t}} + \frac{k_s''(I+J)^{P+\Delta t} \alpha_4''(I+J)^{P+\Delta t} \Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS} \hat{C}_{P_{HS}} \ell_{HS} \right]}$$

$$k_s'(I+J)^P/\ell'^P$$

$$2 \left[ \frac{k_s'(I+J)^{P+\Delta t} \alpha_4'(I+J)^{P+\Delta t} \Delta x'}{\ell'^{P+\Delta t}} + \frac{k_s''(I+J)^{P+\Delta t} \alpha_4''(I+J)^{P+\Delta t} \Delta x''}{\ell''^{P+\Delta t}} - \rho_{HS} \hat{C}_{P_{HS}} \ell_{HS} \right]$$

$$\begin{aligned}
& \left\{ -\frac{1}{6\Delta x'} T_s (I+J-4)^P + \left[ \frac{3}{4\Delta x'} + \frac{1}{3} \alpha_1' (I+J)^P \right] T_s (I+J-3)^P \right. \\
& \quad \left. - \left[ \frac{4}{3\Delta x'} + \frac{3}{2} \alpha_1' (I+J)^P \right] T_s (I+J-2)^P - \left[ \frac{3}{4\Delta x'} - 3\alpha_1' (I+J)^P \right] T_s (I+J-1)^P \right\} \\
& - \left[ \frac{1}{2 \left[ \frac{k_s' (I+J)^P \alpha_4' (I+J)^P \Delta x'}{\ell'^P} + \frac{k_s'' (I+J)^P \alpha_4'' (I+J)^P \Delta x''}{\ell''^P} - \rho_{HS} \hat{C}_{P_{HS}} \ell_{HS} \right]} \right. \\
& \quad \left\{ \frac{k_s' (I+J)^P}{\ell'^P} \left[ \frac{3}{2\Delta x'} - \frac{11}{6} \alpha_1' (I+J)^P - \alpha_2' (I+J)^P \Delta x' \right] + \frac{k_s'' (I+J)^P}{\ell''^P} \left[ \frac{3}{2\Delta x''} \right. \right. \\
& \quad \left. \left. + \frac{11}{6} \alpha_1'' (I+J)^P - \alpha_2'' (I+J)^P \Delta x'' \right] \right\} + \frac{1}{\Delta t} T_s (I+J)^P \\
& \quad + \frac{k_s'' (I+J)^P / \ell''^P}{2 \left[ \frac{k_s' (I+J)^P \alpha_4' (I+J)^P \Delta x'}{\ell'^P} + \frac{k_s'' (I+J)^P \alpha_4'' (I+J)^P \Delta x''}{\ell''^P} - \rho_{HS} \hat{C}_{P_{HS}} \ell_{HS} \right]} \\
& \quad \left\{ \left[ \frac{3}{4\Delta x''} + 3\alpha_1'' (I+J)^P \right] T_s (I+J+1)^P + \left[ \frac{4}{3\Delta x''} - \frac{3}{2} \alpha_1'' (I+J)^P \right] T_s (I+J+2)^P \right. \\
& \quad \left. - \left[ \frac{3}{4\Delta x''} - \frac{1}{3} \alpha_1'' (I+J)^P \right] T_s (I+J+3)^P + \frac{1}{6\Delta x''} T_s (I+J+4)^P \right\} . \tag{5-80}
\end{aligned}$$

At the back surface ( $N = I + J + K$ ).— The back surface boundary condition is

$$\begin{aligned}
& -\frac{1}{\ell''} \left( k_s'' \frac{\partial T_s}{\partial x''} \right)_{N=I+J+K} = \sigma \epsilon_s'' T_s (I+J+K)^4 \\
& - q_B + \rho_{HSP} \hat{C}_{P_{HSP}} \ell_{HSP} \left( \frac{\partial T_s}{\partial t} \right)_{N=I+J+K} . \tag{5-81}
\end{aligned}$$

This equation is combined with the insulation temperature equation following the procedure used for the front surface boundary condition and char layer temperature equation. The resulting modified implicit finite difference equation is

$$\begin{aligned}
 & ZZ_s T_s (I + J + K - 4)^{P + \Delta t} + YZ_s T_s (I + J + K - 3)^{P + \Delta t} \\
 & + XZ_s T_s (I + J + K - 2)^{P + \Delta t} + AZ_s T_s (I + J + K - 1)^{P + \Delta t} \\
 & + BZ_s T_s (I + J + K)^{P + \Delta t} = DZ_s
 \end{aligned} \tag{5-82}$$

where

$$ZZ_s = \frac{k_s''(I+J+K)^{P+\Delta t} / (12 \Delta x''^2 \ell'')}{\left[ \rho_{HSP} \hat{C}_{P_{HSP}} \ell_{HSP} [\alpha_1''(I+J+K)^{P+\Delta t} + \frac{11}{6\Delta x''}] - \alpha_4'' \frac{\alpha_4''(I+J+K)^{P+\Delta t} k_s''(I+J+K)^{P+\Delta t}}{\ell''} \right]} \tag{5-83}$$

$$YZ_s = -4.5 ZZ_s \tag{5-84}$$

$$XZ_s = 8 ZZ_s \tag{5-85}$$

$$AZ_s = -YZ_s \tag{5-86}$$

$$BZ_s = [6\alpha_2''(I+J+K)^{P+\Delta t} \Delta x''^2 - 9] ZZ_s - \frac{1}{\Delta t}$$



$$\begin{aligned}
& - \frac{\sigma \epsilon''_s [T_s (I+J+K)^{P+\Delta t}]^3 [\alpha''_1 (I+J+K)^{P+\Delta t} + \frac{11}{6\Delta x''}] }{2 \left\{ \rho_{HSP} \hat{C}_{P_{HSP}} \ell_{HSP} \left[ \alpha''_1 (I+J+K)^{P+\Delta t} + \frac{11}{6\Delta x''} \right] - \frac{\alpha''_1 (I+J+K)^{P+\Delta t} k''_s (I+J+K)^{P+\Delta t}}{\ell''} \right\}} \\
& \hspace{15em} (5-87)
\end{aligned}$$

$$\begin{aligned}
DZ_s = & - \frac{\alpha''_1 (I+J+K)^{P+\Delta t} + 11/6\Delta x''}{2 \left\{ \rho_{HSP} \hat{C}_{P_{HSP}} \ell_{HSP} \left[ \alpha''_1 (I+J+K)^{P+\Delta t} + \frac{11}{6\Delta x''} \right] - \frac{\alpha''_1 (I+J+K)^{P+\Delta t} k''_s (I+J+K)^{P+\Delta t}}{\ell''} \right\}} \\
& \left\{ q_B^{P+\Delta t} + \frac{\alpha''_3 (I+J+K)^{P+\Delta t} k''_s (I+J+K)^{P+\Delta t} / \ell''}{\alpha''_1 (I+J+K)^{P+\Delta t} + \frac{11}{6\Delta x''}} \right\} \\
& - \frac{\alpha''_1 (I+J+K)^P + 11/6\Delta x''}{2 \left\{ \rho_{HSP} \hat{C}_{P_{HSP}} \ell_{HSP} \left[ \alpha''_1 (I+J+K)^P + \frac{11}{6\Delta x''} \right] - \frac{\alpha''_1 (I+J+K)^P k''_s (I+J+K)^P}{\ell''} \right\}} \\
& \left[ q_B^P + \frac{\alpha''_3 (I+J+K)^P k''_s (I+J+K)^P / \ell''}{\alpha''_1 (I+J+K)^P + 11/6\Delta x''} + \frac{k''_s (I+J+K)^P / \ell''}{\alpha''_1 (I+J+K)^P + 11/6\Delta x''} \right. \\
& \left. \left\{ \frac{1}{6\Delta x''^2} T_s (I+J+K)^P - \frac{3}{4\Delta x''^2} T_s (I+J+K-3)^P + \frac{4}{3\Delta x''^2} T_s (I+J+K-2)^P \right. \right. \\
& \left. \left. + \frac{3}{4\Delta x''^2} T_s (I+J+K-1)^P - \left[ \frac{3}{2\Delta x''^2} - \alpha''_2 (I+J+K)^P \right] T_s (I+J+K)^P \right\} \right. \\
& \left. - \sigma \epsilon''_s [T_s (I+J+K)^P]^4 \right] - \frac{1}{\Delta t} T_s (I+J+K)^P .. \hspace{15em} (5-88)
\end{aligned}$$

## Char Layer Porosity Equation

The differential equation for the char layer porosity is

$$\frac{\partial \eta}{\partial x} + \epsilon_1 \eta + \epsilon_2 + \epsilon_3 \frac{\partial \eta}{\partial t} = 0 . \quad (5-89)$$

The second term in this equation may be much less than 1. Therefore, to assure that the finite difference form of this equation is suitable for obtaining a numerical solution, the first order partial derivative is replaced by a forward difference approximation.

The forward difference approximation of the derivative is obtained from Taylor series expansions at the station  $N$  evaluated at  $N + 1$  and  $N + 2$ . Thus

$$\eta(N + 1) = \eta(N) + \left( \frac{\partial \eta}{\partial x} \right)_N \Delta x + \left( \frac{\partial^2 \eta}{\partial x^2} \right)_N \frac{\Delta x^2}{2} + \left( \frac{\partial^3 \eta}{\partial x^3} \right)_N \frac{\Delta x^3}{6} + \dots \quad (5-90)$$

$$\eta(N + 2) = \eta(N) + 2 \left( \frac{\partial \eta}{\partial x} \right)_N \Delta x + 2 \left( \frac{\partial^2 \eta}{\partial x^2} \right)_N \Delta x^2 + \frac{4}{3} \left( \frac{\partial^3 \eta}{\partial x^3} \right)_N \Delta x^3 + \dots \quad (5-91)$$

Eliminating the second order derivative from this pair of equations and solving for the first order derivative gives:

$$\left( \frac{\partial \eta}{\partial x} \right)_N = [-3\eta(N) + 4\eta(N + 1) - \eta(N + 2)] / 2\Delta x \quad (5-92)$$

which is accurate to terms of the order  $\Delta x^2$ .

Combining Eqs. 5-89 and 5-92 gives

$$\begin{aligned} & [\epsilon_1(N) - \frac{5}{2\Delta x}] \eta(N) + \frac{2}{\Delta x} \eta(N+1) - \frac{1}{2\Delta x} \eta(N+2) \\ & + \epsilon_2(N) + \epsilon_3(N) \left( \frac{\partial \eta}{\partial t} \right)_N = 0 \end{aligned} \quad (5-93)$$

which yields the following modified implicit finite difference equation.

$$\begin{aligned} B(N) \eta(N)^{P + \Delta t} + C(N) \eta(N+1)^{P + \Delta t} + E(N) \eta(N+2)^{P + \Delta t} \\ = D(N) \end{aligned} \quad (5-94)$$

where

$$\begin{aligned} B(N) &= \frac{1}{2\Delta t} [\epsilon_3(N)^P + \epsilon_3(N)^{P + \Delta t}] \\ &+ \frac{1}{2} [\epsilon_1(N)^{P + \Delta t} - \frac{3}{2\Delta x}] \end{aligned} \quad (5-95)$$

$$C(N) = \frac{1}{\Delta x} \quad (5-96)$$

$$E(N) = -\frac{1}{4\Delta x} \quad (5-97)$$

$$\begin{aligned}
D(N) = & -\frac{1}{2} [\epsilon_2(N)^P + \epsilon_2(N)^P + \Delta t] \\
& -\frac{1}{2} \left\{ \epsilon_1(N)^P - \frac{3}{2\Delta x} - \frac{1}{\Delta t} [\epsilon_3(N)^P + \epsilon_3(N)^P + \Delta t] \right\} \eta(N)^P \\
& -\frac{1}{\Delta x} \eta(N+1)^P + \frac{1}{4\Delta x} \eta(N+2)^P .
\end{aligned} \tag{5-98}$$

Equation 5-93 is valid at all stations from  $N = 1$  to  $N = I - 2$ . At  $N = I - 1$  the third term in Eq. 5-93 would contain  $\eta(I + 1)$  which is not defined. The finite difference equation for station  $I - 1$  is obtained in a manner identical to that used to obtain Eq. 5-93 except that the first order derivative is approximated by a two-point forward difference equation. Thus:

$$\left( \frac{\partial \eta}{\partial x} \right)_{N = I - 1} = \frac{\eta(I) - \eta(I - 1)}{\Delta x} \tag{5-99}$$

which is accurate to terms of the order  $\Delta x$ . The resulting modified implicit finite difference equation for station  $I - 1$  is

$$B(I - 1)\eta(I - 1)^P + \Delta t + C(I - 1)\eta(I)^P + \Delta t = D(I - 1) \tag{5-100}$$

where

$$B(I - 1) = \frac{1}{\Delta t} [\epsilon_3(I - 1)^P + \epsilon_3(I - 1)^{P+\Delta t}] + \epsilon_1(I - 1)^{P+\Delta t} - \frac{1}{\Delta x} \quad (5-101)$$

$$C(I - 1) = \frac{1}{\Delta x} \quad (5-102)$$

$$\begin{aligned} D(I - 1) = & - [\epsilon_2(I - 1)^P + \epsilon_2(I - 1)^P] - \{\epsilon_1(I - 1)^P - \frac{1}{\Delta x} \\ & - \frac{1}{\Delta t} [\epsilon_3(I - 1)^P + \epsilon_3(I - 1)^{P + \Delta t}] \} \eta(I - 1)^P \\ & - \frac{1}{\Delta x} \eta(I)^P . \end{aligned} \quad (5-103)$$

The single boundary condition for char layer porosity equation is

$$\eta(I) = \eta_I . \quad (5-104)$$

This identity is used instead of a finite difference equation at station I.

#### Pyrolysis Gas Temperature Equation

The differential equation for the pyrolysis gas temperature is

$$\frac{\partial T}{\partial x} + \beta_1 T + \beta_2 + \beta_3 \frac{\partial T}{\partial t} = 0 . \quad (5-105)$$

The single boundary condition for this equation is

$$T(I) = T_s(I) . \quad (5-106)$$

The forms of the pyrolysis gas temperature equation and its boundary conditions are identical to the char layer porosity equation and boundary condition; therefore, the modified implicit finite difference equation for pyrolysis gas temperature is of the same form as the equations for char layer porosity. Thus for  $1 \leq N \leq I - 2$

$$\begin{aligned} B(N) T(N)^P + \Delta t + C(N) T(N+1)^P + \Delta t + E(N) T(N+2)^P + \Delta t \\ = D(N) \end{aligned} \quad (5-107)$$

where

$$B(N) = \frac{1}{2\Delta t} [\beta_3(N)^P + \beta_3(N)^{P+\Delta t}] + \frac{1}{2} \left[ \beta_1(N)^{P+\Delta t} - \frac{3}{2\Delta x} \right] \quad (5-108)$$

$$C(N) = \frac{1}{\Delta x} \quad (5-109)$$

$$E(N) = -\frac{1}{4\Delta x} \quad (5-110)$$

$$\begin{aligned} D(N) = & -\frac{1}{2} [\beta_2(N)^P + \beta_2(N)^{P+\Delta t}] - \frac{1}{2} \left\{ \beta_1(N)^P - \frac{3}{2\Delta x} \right. \\ & \left. - \frac{1}{\Delta t} [\beta_3(N)^P + \beta_3(N)^{P+\Delta t}] \right\} T(N)^P - \frac{1}{\Delta x} T(N+1)^P + \frac{1}{4\Delta x} T(N+2)^P \end{aligned} \quad (5-111)$$

and, for  $N = I - 1$ ,

$$B(I - 1) T(I - 1)^{P + \Delta t} + C(I - 1) T(I)^{P + \Delta t} = D(I - 1) \quad (5-112)$$

where

$$\begin{aligned} B(I - 1) &= \frac{1}{\Delta t} [\beta_3(I - 1)^P + \beta_3(I - 1)^{P + \Delta t}] \\ &\quad + \beta_1(I - 1)^{P + \Delta t} - \frac{1}{\Delta x} \end{aligned} \quad (5-113)$$

$$C(I - 1) = \frac{1}{\Delta x} \quad (5-114)$$

$$\begin{aligned} D(I - 1) &= - [\beta_2(I - 1)^P + \beta_2(I - 1)^{P + \Delta t}] - \{\beta_1(I - 1)^P \\ &\quad - \frac{1}{\Delta x} - \frac{1}{\Delta t} [\beta_3(I - 1)^P + \beta_3(I - 1)^{P + \Delta t}]\} T(I - 1)^P \\ &\quad - \frac{1}{\Delta x} T(I)^P. \end{aligned} \quad (5-115)$$

The equation applied at  $N = I$  is

$$T(I) = T_s(I) . \quad (5-116)$$

### Pyrolysis Gas Pressure Equation

The differential equation for the pyrolysis gas pressure is

$$\frac{\partial^2 P^2}{\partial x^2} + \gamma_1 \frac{\partial P^2}{\partial x} + \gamma_2 P^2 + \gamma_3 + \gamma_4 \frac{\partial P^2}{\partial t} = 0 . \quad (5-117)$$

Interior stations.— The form of this equation is identical to that of the solid phase temperature equation; hence at interior stations the modified implicit finite difference equations for the pyrolysis gas pressure are written from the finite difference equations for the solid phase temperature as

$$\begin{aligned} A_P(N) P^2(N-1)^{P+\Delta t} + B_P(N) P^2(N)^{P+\Delta t} \\ + C_P(N) P^2(N+1)^{P+\Delta t} = D_P(N) \end{aligned} \quad (5-118)$$

where

$$A_P(N) = \frac{1}{\Delta x^2} - \frac{\gamma_1(N)^{P+\Delta t}}{2\Delta x} \quad (5-119)$$

$$B_P(N) = \gamma_2(N)^{P+\Delta t} - \frac{2}{\Delta x^2} + \frac{1}{\Delta t} [\gamma_4(N)^P + \gamma_4(N)^{P+\Delta t}] \quad (5-120)$$

$$C_P(N) = \frac{1}{\Delta x^2} + \frac{\gamma_1(N)^{P+\Delta t}}{2\Delta x} \quad (5-121)$$



$$\begin{aligned}
D_p(N) = & -\gamma_3(N)^P - \gamma_3(N)^P + \Delta t - \left[ \frac{1}{\Delta x^2} - \frac{\gamma_1(N)^P}{2\Delta x} \right] P^2(N-1)^P \\
& - \left\{ \gamma_2(N)^P - \frac{2}{\Delta x^2} - \frac{1}{\Delta t} [\gamma_4(N)^P + \gamma_4(N)^P + \Delta t] \right\} P^2(N)^P \\
& - \left[ \frac{1}{\Delta x^2} + \frac{\gamma_1(N)^P}{2\Delta x} \right] P^2(N+1)^P .
\end{aligned} \tag{5-122}$$

Front surface boundary condition (N = 1). - The boundary condition for pressure at the front surface is

$$P(1) = P_w \tag{5-123}$$

or

$$P^2(1) = P_w^2 \tag{5-124}$$

which is used instead of a finite difference equation at station 1.

Pyrolysis zone boundary condition (N = I). - The second boundary condition for the pressure equation is the specified pressure gradient at the pyrolysis zone -

$$\left( \frac{\partial P^2}{\partial x} \right)_{N=I} = 2 R_u \ell \left( \frac{\mu T}{K \bar{M}} \right)_{N=I} \dot{m}_g . \tag{5-125}$$

The second order derivative of Eq. 5-117 is written as the first derivative of the gradient of  $P^2$ ,

$$\frac{\partial^2 P^2}{\partial x^2} = \frac{\partial}{\partial x} \left[ \frac{\partial P^2}{\partial x} \right] . \quad (5-126)$$

The derivative of the gradient of  $P^2$  is then approximated by a four-point backward difference expression obtained from Taylor series expansions at the station  $N = I$  evaluated at  $N = I - 1$ ,  $N = I - 2$ , and  $N = I - 3$ . Thus

$$\begin{aligned} \left( \frac{\partial^2 P^2}{\partial x^2} \right)_{N=I} &= \frac{1}{6\Delta x} \left[ 11 \left( \frac{\partial P^2}{\partial x} \right)_{N=I} - 18 \left( \frac{\partial P^2}{\partial x} \right)_{N=I-1} \right. \\ &\quad \left. + 9 \left( \frac{\partial P^2}{\partial x} \right)_{N=I-2} - 2 \left( \frac{\partial P^2}{\partial x} \right)_{N=I-3} \right] . \end{aligned} \quad (5-127)$$

Combining Eq. 5-127 with Eq. 5-117 written for station  $N = I$  gives

$$\begin{aligned} \left[ \frac{11}{6\Delta x} + \gamma_1(I) \right] \left( \frac{\partial P^2}{\partial x} \right)_{N=I} &- \frac{3}{\Delta x} \left( \frac{\partial P^2}{\partial x} \right)_{N=I-1} + \frac{3}{2\Delta x} \left( \frac{\partial P^2}{\partial x} \right)_{N=I-2} \\ &- \frac{1}{3\Delta x} \left( \frac{\partial P^2}{\partial x} \right)_{N=I-3} + \gamma_2(I) P^2(I) + \gamma_3(I) \\ &+ \gamma_4(I) \left( \frac{\partial P^2}{\partial t} \right)_{N=I} = 0 . \end{aligned} \quad (5-128)$$

In Eq. 5-128 the gradient of  $P^2$  at the pyrolysis zone is replaced with Eq. 5-125 and the gradients at neighboring stations are approximated by central difference expressions yielding

$$\begin{aligned}
& \frac{1}{6\Delta x^2} P^2(I-4) - \frac{3}{4\Delta x^2} P^2(I-3) + \frac{4}{3\Delta x^2} P^2(I-2) \\
& + \frac{3}{4\Delta x^2} P^2(I-1) + \left[ \gamma_2(I) - \frac{3}{2\Delta x^2} \right] P^2(I) + \gamma_3(I) \\
& + \left[ \frac{11}{6\Delta x} + \gamma_1(I) \right] 2 \ell R_u \left( \frac{\mu T}{K\bar{M}} \right)_{N=I} \dot{m}_g \\
& + \gamma_4(I) \left( \frac{\partial P^2}{\partial t} \right)_{N=I} = 0 \quad . \quad (5-129)
\end{aligned}$$

The modified implicit finite difference equation for pressure at the pyrolysis zone is obtained from Eq. 5-129 using the procedure previously outlined. Writing the equation,

$$\begin{aligned}
& P_X P^2(I-4)^P + \Delta t + P_Y P^2(I-3)^P + \Delta t + P_Z P^2(I-2)^P + \Delta t \\
& + A_P P^2(I-1)^P + \Delta t + B_P P^2(I)^P + \Delta t \\
& = D_P \quad (5-130)
\end{aligned}$$

where

$$P_X = \frac{1}{12\Delta x^2} \quad (5-131)$$

$$P_Y = - \frac{3}{8\Delta x^2} \quad (5-132)$$

$$PZ = \frac{3}{3\Delta x^2} \quad (5-133)$$

$$AP = - PY \quad (5-134)$$

$$BP = \frac{1}{2\Delta t} [\gamma_4(I)^P + \gamma_4(I)^{P+\Delta t}] + \frac{1}{2} [\gamma_2(I)^P + \Delta t - \frac{3}{2\Delta x^2}] \quad (5-135)$$

$$\begin{aligned} DP = & -\frac{1}{2} [\gamma_3(I)^P + \gamma_3(I)^{P+\Delta t}] - \left[ \frac{11}{6\Delta x} + \gamma_1(I)^P \right] R_u \ell^P \dot{m}_g^P \left( \frac{\mu T}{K\bar{M}} \right)^P_{N=I} \\ & - \left[ \frac{11}{6\Delta x} + \gamma_1(I)^{P+\Delta t} \right] R_u \ell^{P+\Delta t} \dot{m}_g^{P+\Delta t} \left( \frac{\mu T}{K\bar{M}} \right)^{P+\Delta t}_{N=I} \\ & - \frac{1}{12\Delta x^2} P^2(I-4)^P + \frac{3}{8\Delta x^2} P^2(I-3)^P - \frac{3}{3\Delta x^2} P^2(I-2)^P \\ & - \frac{3}{8\Delta x^2} P^2(I-1)^P - \frac{1}{2} \{ \gamma_2(I)^P - \frac{3}{2\Delta x^2} - \frac{1}{\Delta t} [\gamma_4(I)^P \\ & + \gamma_4(I)^{P+\Delta t}] \} P^2(I)^P . \end{aligned} \quad (5-136)$$

#### Chemical Species Conservation Equation

The differential equation for conservation of chemical species is

$$\frac{\partial}{\partial x} \dot{m}_i + \Delta_{1_i} \dot{m}_i + \Delta_{2_i} + \Delta_{3_i} \frac{\partial \dot{m}_i}{\partial t} = 0 . \quad (5-137)$$

The single boundary condition for this equation is

$$(\dot{m}_1)_{N=I} = -M_1 \left( \frac{x_1}{\eta \bar{M}} \right)_{N=I} \dot{m}_g \quad (5-138)$$

This equation and its boundary condition are of the same form as the first order equations and boundary conditions handled previously.

Therefore the modified implicit finite difference equation for conservation of chemical species is written directly as

$$\begin{aligned} B_1(N) \dot{m}_1(N)^{P+\Delta t} + C_1(N) \dot{m}_1(N+1)^{P+\Delta t} \\ + E_1(N) \dot{m}_1(N+2)^{P+\Delta t} = D_1(N) \end{aligned} \quad (5-139)$$

for  $1 \leq N \leq I-2$

where

$$\begin{aligned} B_1(N) &= \frac{1}{2\Delta t} [\Delta_{1_i}(N)^P + \Delta_{1_i}(N)^{P+\Delta t}] \\ &+ \frac{1}{2} [\Delta_{1_i}(N)^{P+\Delta t} - \frac{3}{2\Delta x}] \end{aligned} \quad (5-140)$$

$$C_1(N) = \frac{1}{\Delta x} \quad (5-141)$$

$$E_1(N) = -\frac{1}{4\Delta x} \quad (5-142)$$

$$\begin{aligned}
D_i(N) = & -\frac{1}{2} [\Delta_{2_i}(N)^P + \Delta_{2_i}(N)^{P+\Delta t}] \\
& -\frac{1}{2} \left\{ \Delta_{1_i}(N)^P - \frac{3}{2\Delta x} - \frac{1}{\Delta t} [\Delta_{3_i}(N)^P \right. \\
& \left. + \Delta_{3_i}(N)^{P+\Delta t}] \right\} \dot{m}_i(N)^P - \frac{1}{\Delta x} \dot{m}_i(N+1)^P \\
& + \frac{1}{4\Delta x} \dot{m}_i(N+2)^P
\end{aligned} \tag{5-143}$$

and, for  $N = I - 1$ ,

$$B_i(I-1)\dot{m}_i(I-1)^{P+\Delta t} + C_i(I-1)\dot{m}_i(I)^{P+\Delta t} = D_i(I-1) \tag{5-144}$$

where

$$\begin{aligned}
B_i(I-1) = & \frac{1}{\Delta t} [\Delta_{3_i}(I-1)^P + \Delta_{3_i}(I-1)^{P+\Delta t}] \\
& + \Delta_{1_i}(I-1)^{P+\Delta t} - \frac{1}{\Delta x}
\end{aligned} \tag{5-145}$$

$$C_i(I-1) = \frac{1}{\Delta x} \tag{5-146}$$

$$\begin{aligned}
D_i(I-1) = & -\Delta_{2_i}(I-1)^P - \Delta_{2_i}(I-1)^{P+\Delta t} - \left\{ \Delta_{1_i}(I-1)^P \right. \\
& \left. - \frac{1}{\Delta x} - \frac{1}{\Delta t} [\Delta_{3_i}(I-1)^P + \Delta_{3_i}(I-1)^{P+\Delta t}] \right\} \dot{m}_i(I-1)^P - \frac{1}{\Delta x} \dot{m}_i(I)^P
\end{aligned} \tag{5-147}$$

and, for  $N = I$ ,

$$\dot{m}_i(I) = - M_i \left( \frac{x_i}{\eta \bar{M}} \right)_{N=I} \dot{m}_g. \quad (5-148)$$

## CHAPTER VI

### SOLUTION OF EQUATIONS

The equations formulated to this point are solved on a digital computer. The linearized finite difference equations for solid temperature and pyrolysis gas pressure are solved using the method suggested by L. H. Thomas of the Watson Scientific Computing Laboratory. Thomas' method is presented in Bruce, Peaceman and Rachford (Ref. 32).

Consider the finite difference equations for the solid temperature -  
At the front surface of the char layer ( $N = 1$ ):

$$\begin{aligned} B1_s T_s(1)^{P + \Delta t} + C1_s T_s(2)^{P + \Delta t} + G1_s T_s(3)^{P + \Delta t} \\ + H1_s T_s(4)^{P + \Delta t} + I1_s T_s(5)^{P + \Delta t} = D1_s \end{aligned} \quad (6-1)$$

Within the char layer ( $1 < N < I$ ):

$$A_s(N) T_s(N - 1)^{P + \Delta t} + B_s(N) T_s(N)^{P + \Delta t} + C_s(N) T_s(N + 1)^{P + \Delta t} = D_s(N), \quad (6-2)$$

At the pyrolysis zone ( $N = I$ ):



$$\begin{aligned}
& ZI_s T_s(I-4)^{P+\Delta t} + YI_s T_s(I-3)^{P+\Delta t} + XI_s T_s(I-2)^{P+\Delta t} \\
& + A_s(I) T_s(I-1)^{P+\Delta t} + B_s(I) T_s(I)^{P+\Delta t} + C_s(I) T_s(I+1)^{P+\Delta t} \\
& + EI_s T_s(I+2)^{P+\Delta t} + FI_s T_s(I+3)^{P+\Delta t} + GI_s T_s(I+4)^{P+\Delta t} \\
& = D_s(I)
\end{aligned} \tag{6-3}$$

Within the uncharred material ( $I < N < I + J$ ):

$$A_s(N) T_s(N-1)^{P+\Delta t} + B_s(N) T_s(N)^{P+\Delta t} + C_s(N) T_s(N+1)^{P+\Delta t} = D_s(N) \tag{6-4}$$

At the uncharred layer-insulation layer interface ( $N = I + J$ ):

$$\begin{aligned}
& ZP_s T_s(I+J-4)^{P+\Delta t} + YP_s T_s(I+J-3)^{P+\Delta t} + XP_s T_s(I+J-2)^{P+\Delta t} \\
& + AP_s T_s(I+J-1)^{P+\Delta t} + BP_s T_s(I+J)^{P+\Delta t} \\
& + CP_s T_s(I+J+1)^{P+\Delta t} + EP_s T_s(I+J+2)^{P+\Delta t} \\
& + FP_s T_s(I+J+3)^{P+\Delta t} + GP_s T_s(I+J+4)^{P+\Delta t} \\
& = D_s(I+J)
\end{aligned} \tag{6-5}$$

Within the insulation layer ( $I + J < N < I + J + K$ ):

$$A_s(N) T_s(N-1)^{P+\Delta t} + B_s(N) T_s(N)^{P+\Delta t} + C_s(N) T_s(N+1)^{P+\Delta t} = D_s(N) \quad (6-6)$$

At the back surface of the insulation ( $N = I + J + K$ ):

$$\begin{aligned} & ZZ_s T_s(I + J + K - 4)^{P+\Delta t} + YZ_s T_s(I + J + K - 3)^{P+\Delta t} \\ & + XZ_s T_s(I + J + K - 2)^{P+\Delta t} + Az_s T_s(I + J + K - 1)^{P+\Delta t} \\ & + Bz_s T_s(I + J + K)^{P+\Delta t} = Dz_s . \end{aligned} \quad (6-7)$$

Equation 6-1 is combined with Eq. 6-2 written for stations 2, 3, and 4 to obtain an equation relating  $T_s(1)$  and  $T_s(2)$  which is valid at station 1. Also Eq. 6-7 is combined with Eq. 6-6 written for stations  $(I + J + K - 4)$ ,  $(I + J + K - 3)$ , and  $(I + J + K - 2)$  to obtain an equation relating  $T_s(I + J + K - 1)$  and  $T_s(I + J + K)$  which is valid at station  $(I + J + K)$ . Similarly, the interface equations are combined with equations for neighboring stations to obtain equations relating the interface temperature to the temperature at the two adjacent stations. The resulting set of equations is tri-diagonal and may be written as

$$\left. \begin{aligned}
 &B_s(1) T_s(1)^{P + \Delta t} + C_s(1) T_s(2)^{P + \Delta t} = D_s(1) & N = 1 \\
 &A_s(N) T_s(N-1)^{P + \Delta t} + B_s(N) T_s(N)^{P + \Delta t} \\
 &\quad + C_s(N) T_s(N+1)^{P + \Delta t} = D_s(N) & 1 < N < I + J + K \\
 &A_s(I + J + K) T_s(I + J + K - 1)^{P + \Delta t} + B_s(I + J + K) \\
 &\quad T_s(I + K + K)^{P + \Delta t} = D_s(I + J + K) & N = I + J + K
 \end{aligned} \right\} (6-8)$$

Thomas' method for solving Eq. 6-8 is equivalent to Gaussian elimination, but it avoids the error growth associated with the back solution of the elimination method and it minimizes the storage requirements for machine calculations. Ref. 30 summarizes the method as follows: For the set of Eqs. 6-8

let

$$\left. \begin{aligned}
 &W(1) = B_s(1) \\
 &W(N) = B_s(N) - A_s(N) B(N-1) & 2 \leq N \leq I + J + K \\
 &B(N) = C_s(N) / W(N) & 1 \leq N \leq I + J + K - 1
 \end{aligned} \right\} (6-9)$$

and

$$\left. \begin{aligned} G(1) &= D_s(1)/W(1) \\ G(N) &= [D_s(N) - A_s(N) G(N-1)]/W(N) \quad 2 \leq N \leq I + J + K. \end{aligned} \right\} (6-10)$$

The solution is

$$\left. \begin{aligned} T_s(I + J + K)^{P + \Delta t} &= G(I + J + K) \\ T_s(N)^{P + \Delta t} &= G(N) - B(N) T_s(N + 1)^{P + \Delta t} \quad 1 \leq N \leq I + J + K - 1. \end{aligned} \right\} (6-11)$$

The finite difference equations for the pyrolysis gas pressure within the char layer are of the same form as those for the solid temperature, hence they are solved in the same manner.

The finite difference equations for the pyrolysis gas temperature, conservation of chemical species, and char layer porosity differ from the solid temperature and gas pressure equations in that the equations at internal stations are not symmetric with respect to the diagonal elements. Treatment of the set of equations for the pyrolysis gas temperature is shown as an example.

The set of finite difference equations for the pyrolysis gas temperature is

$$\left. \begin{aligned} B(N) T(N)^{P + \Delta t} + C(N) T(N + 1)^{P + \Delta t} + E(N) T(N + 2)^{P + \Delta t} \\ = D(N) \quad 1 \leq N \leq I - 2 \\ B(I - 1) T(I - 1)^{P + \Delta t} + C(I - 1) T(I)^{P + \Delta t} = D(I - 1) \\ T(I)^{P + \Delta t} = T_s(I)^{P + \Delta t} \end{aligned} \right\} (6-12)$$

Since each equation relates the temperature at a station to the temperature at forward stations the solution to this set of equations is obtained directly by working from the pyrolysis zone toward the front surface. Thus

$$\left. \begin{aligned}
 T(I)^P + \Delta t &= T_s(I)^P + \Delta t \\
 T(I-1)^P + \Delta t &= [D(I-1) - C(I-1) T(I)^P + \Delta t] / B(I-1) \\
 T(N)^P + \Delta t &= [D(N) - C(N) T(N+1)^P + \Delta t \\
 &\quad - E(N) T(N+2)^P + \Delta t] / B(N) \quad 1 \leq N \leq I-2.
 \end{aligned} \right\} (6-13)$$

The differential equation for conservation of mass is solved by numerical integration from the pyrolysis zone, where the mass flow rate of pyrolysis gases is known, to the front surface of the char layer. The transformed mass conservation equation is written in integral form as

$$\int_a^b \frac{\partial}{\partial x} (\dot{m}) \, dx = \ell \int_a^b \left[ \frac{\partial}{\partial t} (\eta \rho) - \eta \sum_i R_{T_i} M_i - v_c \frac{\partial}{\partial x} (\eta \rho) \right] dx \quad (6-14)$$

The term on the left side of this equation is integrated immediately to obtain

$$\dot{m}_b = \dot{m}_a + \ell \int_a^b \left[ \frac{\partial}{\partial t} (\eta \rho) - \eta \sum_i R_{T_i} M_i - v_c \frac{\partial}{\partial x} (\eta \rho) \right] dx \quad (6-15)$$

If the lower limit of integration is station N and the upper limit is the pyrolysis zone (N = I), Eq. 6-14 becomes

$$\begin{aligned} \dot{m}(N) = \dot{m}(I) - \ell \int_{x(N)}^I \left[ \frac{\partial}{\partial t} (\eta \rho) - \eta \sum_i R_{T_i} M_i \right] dx \\ + \int_{x(N)}^I V_c \frac{\partial}{\partial x} (\eta \rho) dx, \end{aligned} \quad (6-16)$$

Equation (4-9) for  $V_c$  is used in the second integral in Eq. 6-16 and the result is integrated by parts to obtain

$$\begin{aligned} \dot{m}(N) = \dot{m}(I) - \ell \int_{x(N)}^I \left[ \frac{\partial}{\partial t} (\eta \rho) - \eta \sum_i R_{T_i} M_i \right] dx \\ + V_c(I) \eta(I) \rho(I) - V_c(N) \eta(N) \rho(N) \\ - (\dot{m}_g / \Delta \rho - \dot{m}_s / \rho_{s_o}) \int_{x(N)}^I \eta \rho dx. \end{aligned} \quad (6-17)$$

These sets of equations were programmed for solution by a digital computer. As these equations are quasi-linear it is necessary to iterate to obtain a solution. A total of nine homogeneous and heterogeneous chemical reactions involving 12 gaseous species plus solid carbon were considered.

Table 1 shows the chemical reactions, kinetics data, and rate laws included in the program. Table 2 gives a set of thermophysical properties data for a typical ablation material (low density phenolic-

nylon) which was input to this program. Data for viscosity and thermal conductivity of the gaseous species were obtained from Svehla (Ref. 33). The viscosity and thermal conductivity of the pyrolysis gas mixture are computed using the method presented by Brokaw in Ref. 34. Specific heat and enthalpy data for the gaseous species and enthalpy data for the char layer (solid carbon) were obtained from McBride and Bauer (Refs. 35 and 36).

Appendix A presents a general flow chart of the program. Appendix B gives program usage instructions including definitions of the input terminology. The program Fortran 600 statements are presented in Appendix C. Appendix D defines the program terminology.

Table 1.- Chemical Reactions Involving Pyrolysis Gases and Char (Pike, Ref. 37).

(General reaction:  $aA + bB + \dots \xrightleftharpoons[k_r]{k_f} nN + oO + \dots$ )

$$k = A \exp (-B/T)$$

Reaction	Type	Rate law	Frequency factor, A	Activation energy, B °K
1. $\text{CH}_4 \rightarrow \frac{1}{2} \text{C}_2\text{H}_6 + \frac{1}{2} \text{H}_2$	Homogeneous	$k_f A$	$7.6 \times 10^{14}$	$4.775 \times 10^4$
2. $\text{C}_2\text{H}_6 \rightarrow \text{C}_2\text{H}_4 + \text{H}_2$	Homogeneous	$k_f A$	$3.14 \times 10^{15}$	$3.019 \times 10^4$
3. $\text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_2 + \text{H}_2$	Homogeneous	$k_f A$	$2.57 \times 10^8$	$1.157 \times 10^5$
4. $\text{C}_2\text{H}_2 \rightarrow 2\text{C} + \text{H}_2$	Homogeneous	$k_f A^2$	$2.14 \times 10^{10}$	$2.009 \times 10^4$
5. $\text{C}_6\text{H}_6 \rightarrow 6\text{C} + 3\text{H}_2$	Homogeneous	$k_f A$	$1.4 \times 10^{11}$	$2.622 \times 10^4$
6. $\text{C} + \text{CO}_2 \rightarrow 2\text{CO}$	Heterogeneous	$k_f B$	$1.2 \times 10^{12}$	$4.282 \times 10^4$
7. $\text{C} + \text{H}_2\text{O} \rightarrow \text{CO} + \text{H}_2$	Heterogeneous	$k_f B$	$9.26 \times 10^3$	$3.524 \times 10^4$
8. $\text{NH}_3 \rightarrow \frac{1}{2} \text{N}_2 + 1.5\text{H}_2$	Homogeneous	$k_f A$	$2.86 \times 10^6$	$3.055 \times 10^4$
9. $\text{NH}_3 + \text{C} \rightarrow \text{HCN} + \text{H}_2$	Heterogeneous	$k_f A$	$8.78 \times 10^6$	$3.885 \times 10^4$



Table 2.- Thermophysical Properties of Low-Density  
Phenolic-Nylon Ablation Material (Dow and Bush,  
Ref. 38).

### Char

Oxidation kinetics (first order) -	
Specific reaction rate constant, $\text{kg/m}^2\text{-sec-atm}$ . . . .	$4.90 \times 10^{10}$
Activation energy, $^{\circ}\text{K}$ . . . . .	$4.25 \times 10^4$
Mass of char removed per mass of oxygen reaching	
the surface. . . . .	0.75
Heat of combustion, $\text{J/kg}$ . . . . .	$1.20 \times 10^7$
Heat of sublimation, $\text{J/kg}$ . . . . .	$5.00 \times 10^7$
Surface emissivity . . . . .	0.80
Theoretical density, $\text{kg/m}^3$ . . . . .	$1.43 \times 10^3$
Porosity at pyrolysis zone . . . . .	0.85
Proportionality constant in equation for gas	
char heat transfer coefficient, $1/\text{m}$ . . . . .	$1.00 \times 10^3$
Permeability, $\text{m}^2$ . . . . .	$1.00 \times 10^{-9}$
Thermal conductivity, $\text{W/m-}^{\circ}\text{K}$ , at temperature of -	
278 $^{\circ}\text{K}$ . . . . .	0.16
833 $^{\circ}\text{K}$ . . . . .	0.16
1110 $^{\circ}\text{K}$ . . . . .	0.50
1390 $^{\circ}\text{K}$ . . . . .	1.22
1670 $^{\circ}\text{K}$ . . . . .	1.87
1940 $^{\circ}\text{K}$ . . . . .	2.65
2220 $^{\circ}\text{K}$ . . . . .	3.74
2500 $^{\circ}\text{K}$ . . . . .	4.75
2780 $^{\circ}\text{K}$ . . . . .	6.24
3050 $^{\circ}\text{K}$ . . . . .	7.66

### Uncharred Material

Pyrolysis kinetics -	
Specific reaction rate constant, $\text{kg/m}^2\text{-sec-atm}$ . . . .	$7.74 \times 10^6$
Activation energy, $^{\circ}\text{K}$ . . . . .	$1.289 \times 10^4$
Effective heat of pyrolysis, $\text{J/kg}$ . . . . .	$1.28 \times 10^6$
Specific heat, $\text{J/kg-}^{\circ}\text{K}$ , at temperature of -	
311 $^{\circ}\text{K}$ . . . . .	$1.51 \times 10^3$
367 $^{\circ}\text{K}$ . . . . .	$1.80 \times 10^3$
423 $^{\circ}\text{K}$ . . . . .	$2.07 \times 10^3$
478 $^{\circ}\text{K}$ . . . . .	$2.24 \times 10^3$
533 $^{\circ}\text{K}$ . . . . .	$2.28 \times 10^3$
589 $^{\circ}\text{K}$ . . . . .	$2.28 \times 10^3$
Thermal conductivity, $\text{W/m-}^{\circ}\text{K}$ , at temperature of -	
300 $^{\circ}\text{K}$ . . . . .	0.080
390 $^{\circ}\text{K}$ . . . . .	0.084
500 $^{\circ}\text{K}$ . . . . .	0.088
610 $^{\circ}\text{K}$ . . . . .	0.092
710 $^{\circ}\text{K}$ . . . . .	0.094

Table 2.- Concluded

Initial composition of pyrolysis gases - mole  
fraction of chemical species at pyrolysis zone -

CH <sub>4</sub>	0.0
H <sub>2</sub>	0.294
C <sub>2</sub> H <sub>4</sub>	0.0
C <sub>2</sub> H <sub>2</sub>	0.0
CO	0.59
H <sub>2</sub> O	0.0
NH <sub>3</sub>	0.0
N <sub>2</sub>	0.009
CO <sub>2</sub>	0.0
HCN	0.0
C <sub>2</sub> H <sub>6</sub>	0.0
C <sub>6</sub> H <sub>6</sub>	0.107

## CHAPTER VII

### ANALYSIS VERIFICATION

The developments presented in Chapters IV and V represent the usual approach to obtaining numerical solutions to differential equations of engineering and physics. However, the system of algebraic equations resulting from that procedure were found to be unstable for certain conditions. This problem was overcome by including a graded finite difference spacing in the char layer and the uncharred layer and by rewriting the char layer equation (Eq. 4-12) to include the complete term,  $H_A(T_s - T)$ , in the " $\alpha_3$ " term. The graded finite difference spacing was used to reduce the spacing in regions of large gradients (near the front surface of the char layer and in the uncharred layer, near the pyrolysis zone). Numerical solutions have been compared with exact solutions for a number of simplified cases. The results of these comparisons are presented in the following sections.

#### Comparison of Numerical Results With

#### Exact Solutions

The set of equations whose solution is presented here is too complex to obtain an exact solution for a general case to check the accuracy of the numerical analysis. However, exact solutions have been obtained for a number of simplified problems to serve as a check of results obtained using the finite difference equations.

The exact solutions employed here are for the following problems

- (1) The Laplace equation for  $P^2$ .
- (2) Flow of a constant property, incompressible fluid through an isothermal slab.
- (3) Heat sink case (flat plate subjected to surface heating).
- (4) Quasi-steady ablation case.

Laplace equation for  $P^2$ .- The differential equation governing the pyrolysis gas pressure in the char layer is given by Eq. 4-47

$$\frac{\partial^2 P^2}{\partial x^2} + \gamma_1 \frac{\partial P^2}{\partial x} + \gamma_2 P^2 + \gamma_3 + \gamma_4 \frac{\partial P^2}{\partial t} = 0 . \quad (7-1)$$

where the coefficients are not constant. The boundary and initial conditions imposed on  $P^2$  are

$$\left. \begin{aligned} P^2_{x=0} &= P^2_w \\ \left( \frac{\partial P^2}{\partial x} \right)_{x=1} &= 2 \ell R_u \left( \frac{\mu T}{K \bar{M}} \right)_{x=1} \dot{m}_g \\ P^2(x, 0) &= P^2_{w,0} \end{aligned} \right\} \quad (7-2)$$

Equation 7-1 written for the idealized case of flow of a constant property, incompressible fluid through an isothermal slab with the fluid and slab in thermal equilibrium reduces to the Laplace equation,

$$\nabla^2 P^2 = 0.$$

The solution of the Laplace equation subject to Eq. 7-2 is

$$P = \left[ \frac{2\mu \ell R_u T \dot{m}_g}{K\bar{M}} x + P_w^2 \right]^{1/2} \quad (7-3)$$

Results obtained from Eq. 7-3 were compared with the results from the numerical analysis for this idealized case. These results are shown in Fig. 5a and 5b for  $P_w = 0.01$  and  $P_w = 0.1$  Atm, respectively. Note that the error is less than 0.02% for each set of results.

Flow of a constant property incompressible fluid through an isothermal slab.— The differential equation governing the pyrolysis gas temperature is given by Eq. 4-30

$$\frac{\partial T}{\partial x} + \beta_1 T + \beta_2 + \beta_3 \frac{\partial T}{\partial t} = 0 \quad (7-4)$$

where the coefficients are not constant. The boundary and initial conditions imposed on  $T$  are

$$\left. \begin{aligned} T(1,t) &= T_{s_{x=1}} \quad \text{for } t > 0 \\ T(x,0) &= T_{s_0} \end{aligned} \right\} \quad (7-5)$$

The governing energy equation for the idealized case of a constant property incompressible fluid flowing from a reservoir of specified temperature through an isothermal slab (Fig. 6) is

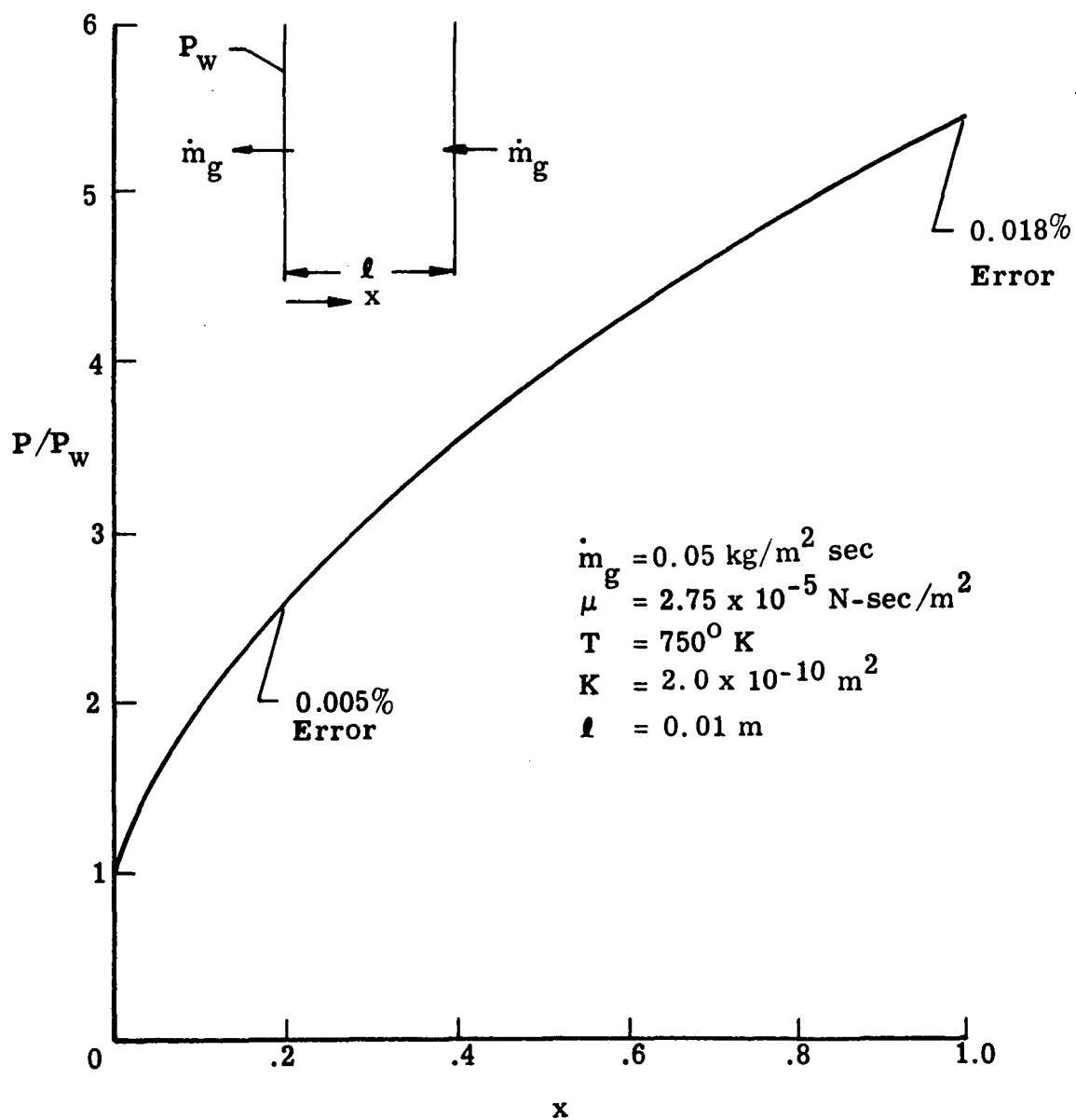


Figure 5a.- Comparison of results for numerical and exact solutions to the Laplace equation for  $P^2$  with  $P_w = 0.01 \text{ ATM}$ .

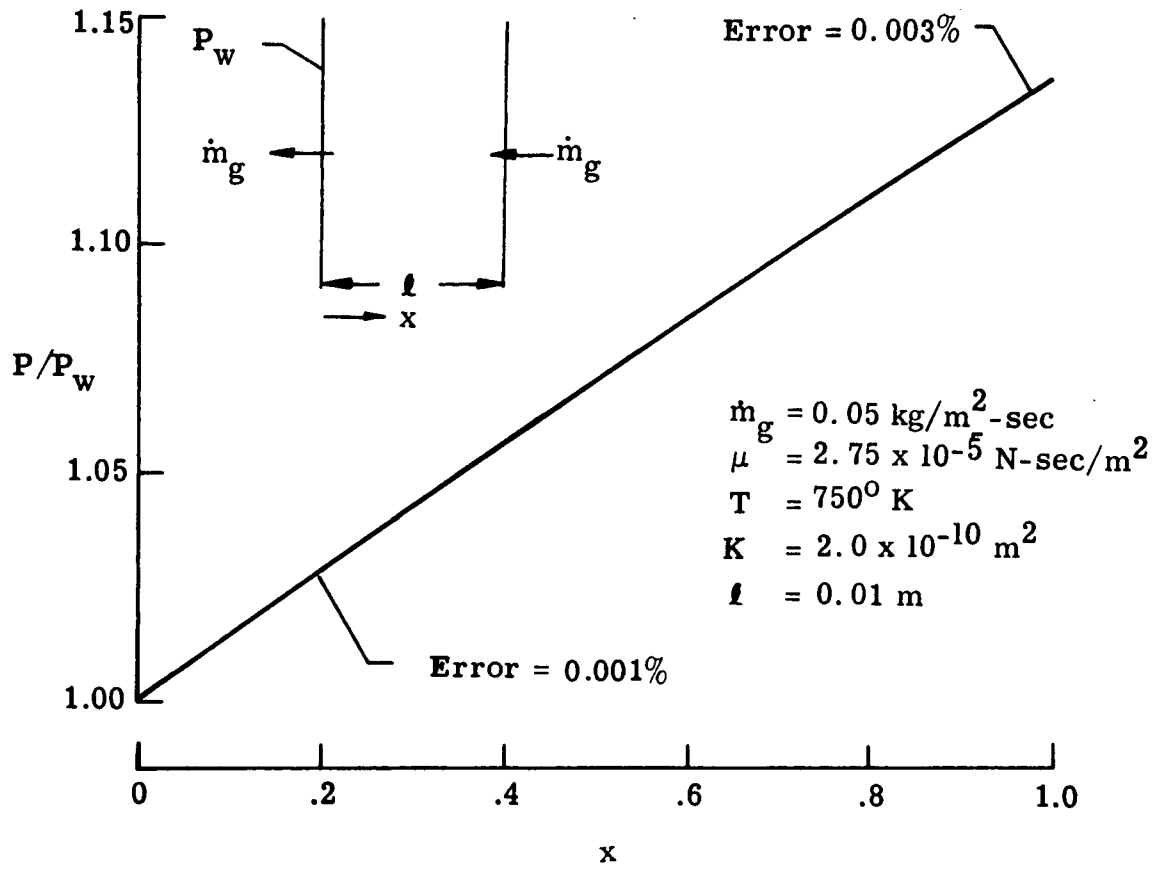


Figure 5b.- Comparison of results for numerical and exact solutions to the Laplace equation for  $P^2$  with  $P_w = 0.1 \text{ ATM.}$

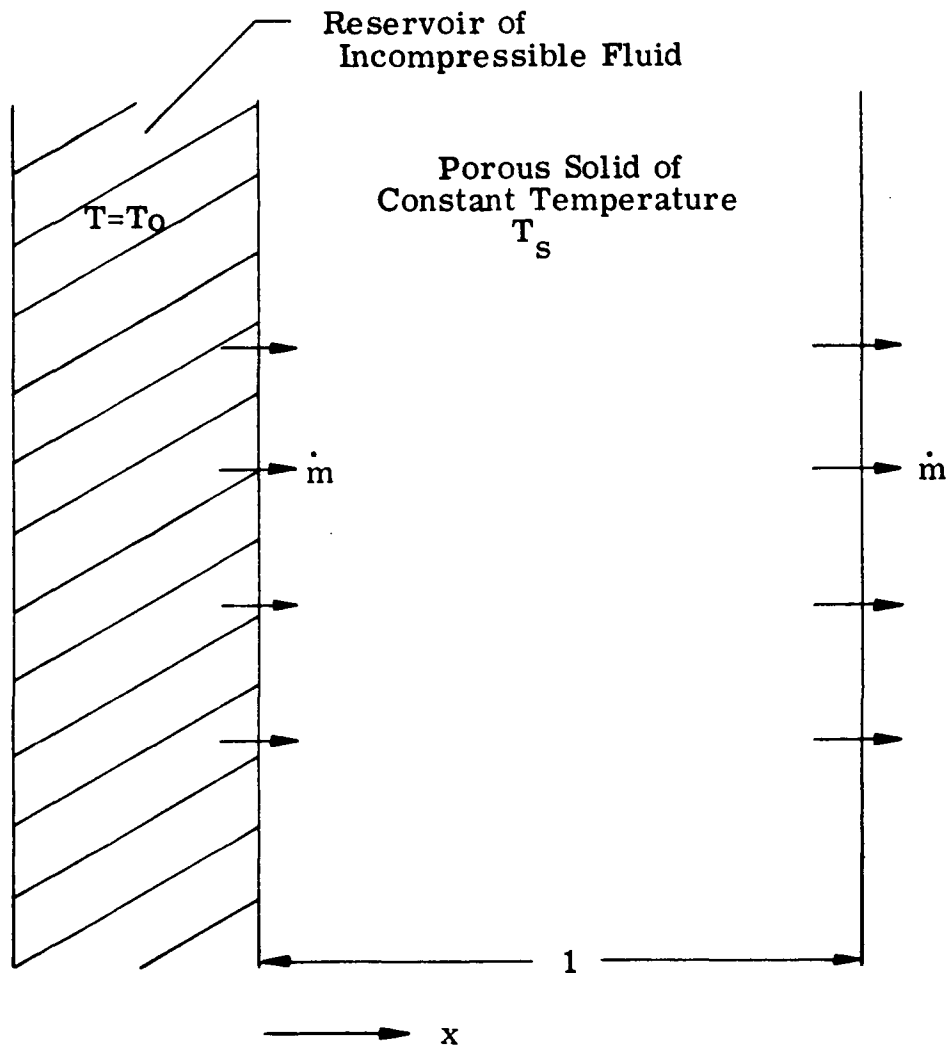


Figure 6.- Flow of constant property incompressible fluid through an isothermal slab.



$$\frac{\partial T'}{\partial x'} + AT' + \frac{\partial T'}{\partial t} = 0 \quad (7-6)$$

where

$$\left. \begin{aligned} T' &= \frac{T - T_s}{T_0 - T_s} \\ x' &= x\ell/v \\ A &= \frac{H_A}{\eta\rho C_p} \end{aligned} \right\} \quad (7-7)$$

and the boundary and initial conditions for  $T'$  are

$$\left. \begin{aligned} T'(0,t) &= 1.0 \quad \text{for } t > 0 \\ T'(x',0) &= 0. \end{aligned} \right\} \quad (7-8)$$

To solve this set of equations the Laplace transform of  $T$  defined by

$$P = \int_0^\infty e^{-St} T'(x',t) dt \quad (7-9)$$

is introduced. Equations 7-6 and 7-8 become

$$\left. \begin{aligned} \frac{\partial P}{\partial x'} + (A + S) P &= 0 \\ P(0, t) &= 1./S \\ P(x', 0) &= 0. \end{aligned} \right\} \quad (7-10)$$

The solution to Eq. 7-10 is

$$P = \exp(-Ax') \frac{1}{S} \exp(-Sx'). \quad (7-11)$$

Performing the reverse transformation of Eq. 7-11 gives the solution to Eq. 7-6 and 7-8 as

$$T'(x', t) = \exp(-Ax') S(t - x') \quad (7-12)$$

where

$$S(t - x') = \begin{cases} 0 & \text{when } 0 < t < x' \\ 1 & \text{when } t > x' \end{cases} \quad (7-13)$$

This is just the mathematical expression for a traveling wave of diminishing strength.

This idealized case was solved with  $A = 1.0$  and  $l/v = 1.0$  using the finite difference equations. These numerical results are compared with the exact solution obtained from Eqs. 7-12 and 7-13 in

Figs. 7a and 7b for dimensionless finite difference spacings of 0.001 and 0.01. The comparison with the transient results is favorable for the fine spacing, but, as expected, the ability to indicate a step change decreases with increased grid spacing. The steady profile solutions differ by less than 0.02% for each case.

Heat sink case.— The exact solution for the temperature response of a flat plate subjected to a constant surface heating is (Carslaw and Jaeger, Ref. 39)

$$T_s = T_{s0} + q(\ell + \ell')/k_s \left\{ \frac{k_s t}{\rho_s \hat{C}_p (\ell + \ell')^2} + \frac{1}{2} (1 - x)^2 - \frac{1}{6} - \frac{2}{\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \cos [n\pi(1 - x)] \exp \left[ n^2 \pi^2 \frac{k_s t}{\rho_s \hat{C}_p (\ell + \ell')^2} \right] \right\}. \quad (7-14)$$

This equation was used to determine the transient response of a flat plate using the heating rate and material properties listed in Table 3. Solutions were obtained for the same problem using the finite-difference equations.

Figure 8 shows a comparison between the numerical results and the exact solution for time steps of 0.01 and 0.1 second. It can be seen that the error at  $t = 2.0$  second is less than 2.0% for the large time step of 0.1 second.

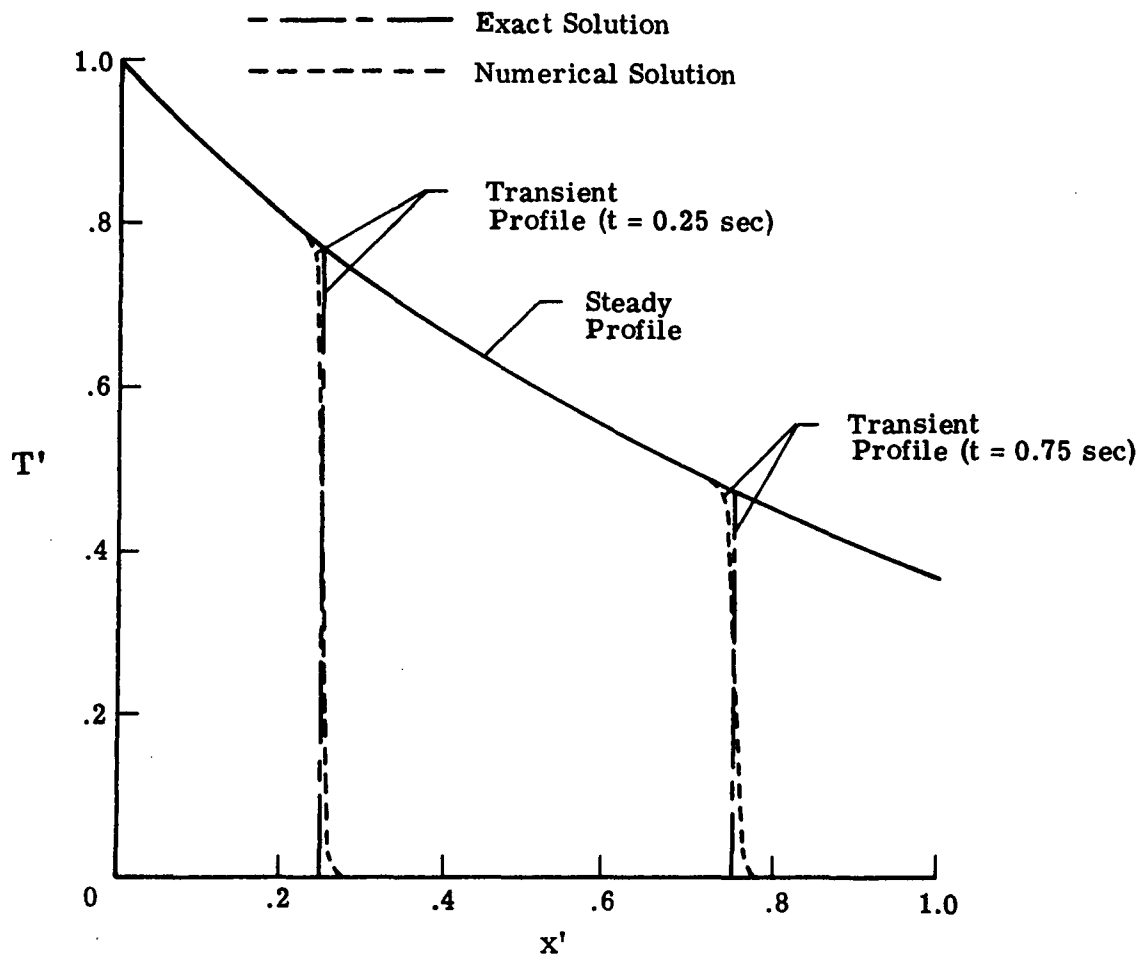


Figure 7a.- Comparison of numerical results with the exact solution for flow of a constant property incompressible fluid through an isothermal slab with  $\Delta x = .001$ .

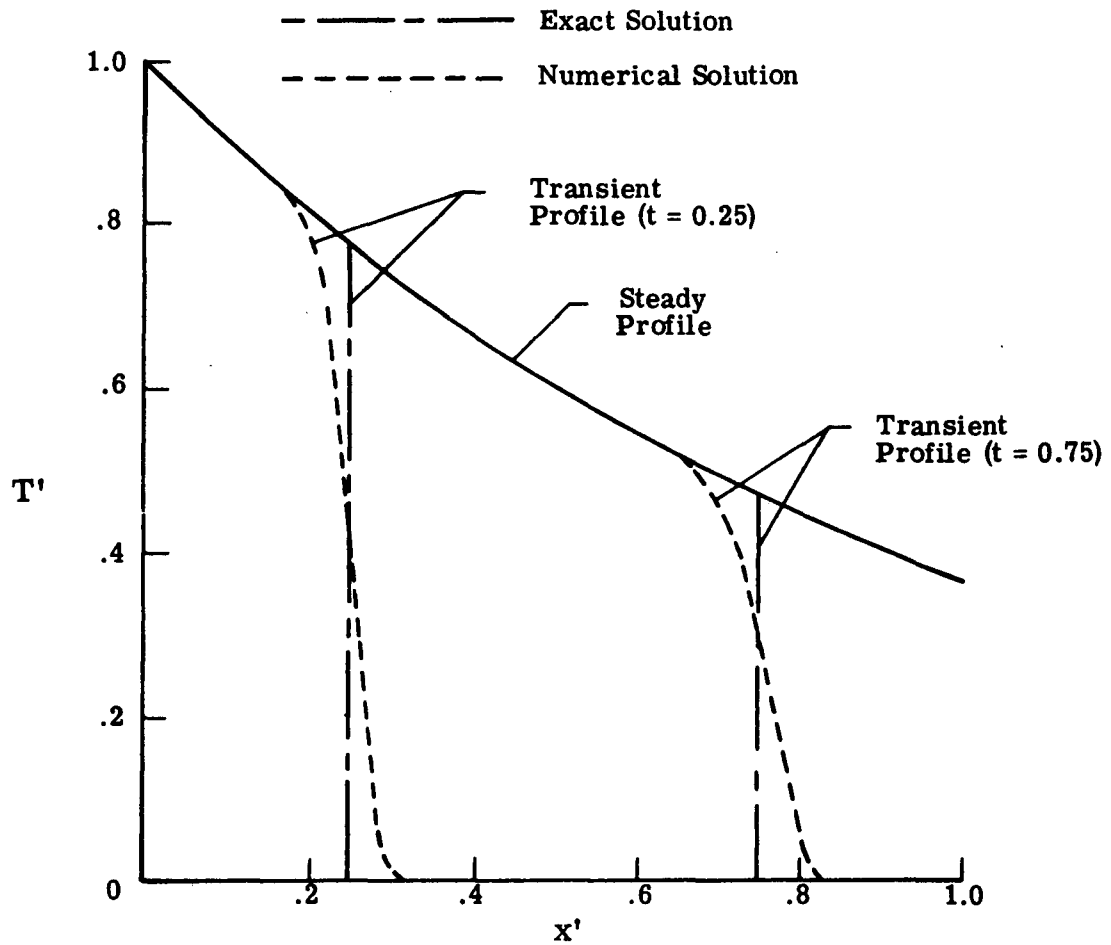


Figure 7b.- Comparison of numerical results with the exact solution for flow of a constant property incompressible fluid through an isothermal slab with  $\Delta X = .01$ .

Table 3.- Inputs Used in Exact Solution to  
Heat Sink Case.

Quantity	Value
$q$	$1. \times 10^6 \text{ W/m}^2$
$l$	$0.01 \text{ m}$
$l'$	$0.01 \text{ m}$
$k_s$	$0.624 \text{ W/m}^2\text{-}^\circ\text{K}$
$\rho_s$	$2140 \text{ kg/m}^3$
$\hat{C}_{p_s}$	$715.16 \text{ J/kg-}^\circ\text{K}$
$T_{s_o}$	$300^\circ \text{ K}$

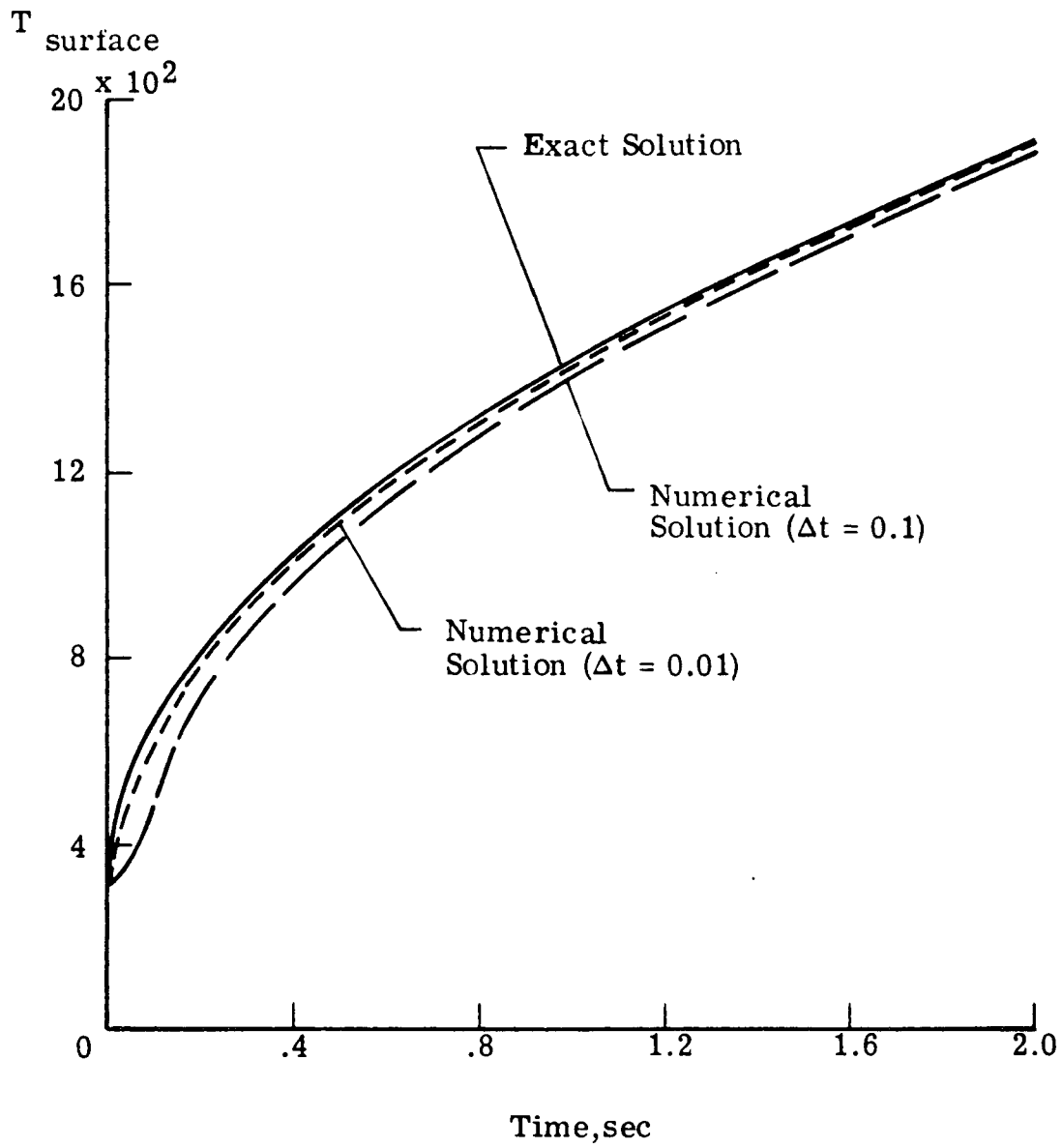


Figure 8.- Comparison of numerical results with the exact solution for the heat sink problem.

Quasi-steady ablation case.— A quasi-steady-state ablating system is one in which the pyrolysis interface and the front surface recede at the same rate, that is it maintains a constant char thickness. If in addition the pyrolysis gases are inert, incompressible, and in local thermal equilibrium with the char layer, material properties of the system are uniform and independent of temperature, there are no energy sources, viscous dissipation or diffusion and conditions exist such that no energy is transferred into the uncharred layer, an exact solution to the governing mathematical equations can be obtained.

The equation governing the char layer temperature is (Eq. 4-11)

$$\begin{aligned}
 (1 - \eta) \frac{\rho_s C_{P_s}}{M_s} \left[ \frac{\partial T_s}{\partial t} - v_c \frac{\partial T_s}{\partial x} \right] &= \frac{k_s}{\ell^2} \frac{\partial^2 T_s}{\partial x^2} \\
 &+ \frac{1}{\ell^2} \frac{\partial k_s}{\partial x} \frac{\partial T_s}{\partial x} - H_A (T_s - T) + \eta R_s H(T)_s \\
 &+ \eta R_{h_s} H_s - \eta \sum_r r_h^{(r)} \Delta H^{(r)} + (1 - \eta) (A - \epsilon) \\
 &+ (1 - \eta) q_s''' + \frac{\rho_s H_s}{M_s} \left( \frac{\partial \eta}{\partial x} - v_c \frac{\partial \eta}{\partial x} \right). \quad (7-15)
 \end{aligned}$$

The equation governing the pyrolysis gas temperature is (Eq. 4-27)

$$\begin{aligned}
 \eta(v/\ell - v_c) \left[ \sum_i \frac{\rho_i C_{P_i}}{M_i} - R_u \sum_i \rho_i / M_i \right] \frac{\partial T}{\partial x} &- H_A (T_s - T) \\
 - \eta R_u \left[ \frac{\rho}{\eta \bar{M}} \left( \frac{\partial \eta}{\partial t} - v_c \frac{\partial \eta}{\partial x} \right) + \frac{\partial}{\partial t} \left( \sum_i \rho_i / M_i \right) + (v/\ell \right.
 \end{aligned}$$



$$\begin{aligned}
& - v_c) \frac{\partial}{\partial x} \left( \sum_i \rho_i / M_i \right) \Big] T + \eta \sum_i H_i R_{T_i} - \frac{1}{\ell} \sum_i H_i \frac{\partial}{\partial x} J_i \\
& - \frac{v^2}{2} \sum_i R_{T_i} M_i - \frac{\tau_{xx}}{\ell^3} \frac{\partial v}{\partial x} - \eta \sum_i \frac{J_i g_i}{M_i} + \frac{1}{\ell^2} \frac{\partial}{\partial x} q_x \\
& - \eta (A' - \epsilon') + \eta R_s H(T)_s + \eta R_{h_s} H_s \\
& - \eta \sum_r \sum_h r(r) \Delta H(r) + \eta \left( \sum_i \frac{\rho_i C_{P_i}}{M_i} - R_u \sum_i \rho_i / M_i \right) \frac{\partial T}{\partial t} = 0, \quad (7-16)
\end{aligned}$$

With quasi-steady-state ablation,  $\ell$ ,  $\dot{m}_g$ , and  $\dot{m}_s$  are constant and

$$\left. \begin{aligned}
\dot{m}_g / \Delta \rho &= \dot{m}_s / \rho_{s_0} \\
\frac{\partial T_s}{\partial t} &= 0 \\
\frac{\partial T}{\partial t} &= 0
\end{aligned} \right\} \quad (7-17)$$

Using Eq. 7-17 with the assumptions of no chemical reactions, incompressible pyrolysis gases, constant material properties, and no energy sources, viscous dissipation, or diffusion, Eq. 7-15 and 7-16 reduce to

$$\frac{\partial^2 T_s}{\partial x^2} + \frac{\ell}{k_s} \hat{C}_{P_s} \dot{m}_s \frac{\partial T_s}{\partial x} - \frac{\ell^2}{k_s} H_A (T_s - T) = 0 \quad (7-18)$$

$$\eta(v/\ell - \dot{m}_s/\rho_{s_o} \ell) \left[ \rho \hat{C}_P - R_u \sum_i \rho_i/M_i \right] \frac{\partial T}{\partial x} - H_A(T_s - T) = 0, \quad (7-19)$$

Equations 7-18 and 7-19 are combined to eliminate the term,  $H_A(T_s - T)$ , thus

$$\begin{aligned} \frac{\partial^2 T_s}{\partial x^2} + \frac{\ell}{k_s} \left[ \hat{C}_{P_s} \dot{m}_s \frac{\partial T_s}{\partial x} - \eta (v - \dot{m}_s/\rho_{s_o}) (\rho \hat{C}_P \right. \\ \left. - R_u \sum_i (\rho_i/M_i) \frac{\partial T}{\partial x}) \right] = 0, \end{aligned} \quad (7-20)$$

Invoking the assumption of local thermal equilibrium between the pyrolysis gases and char layer  $\left\{ T = T_s \text{ and } \frac{\partial T}{\partial x} = \frac{\partial T_s}{\partial x} \right\}$  gives

$$\frac{\partial^2 T_s}{\partial x^2} + D \frac{\partial T_s}{\partial x} = 0 \quad (7-21)$$

where

$$D = \frac{\ell}{k_s} \left[ \dot{m}_s \hat{C}_{P_s} + \left( \dot{m}_g + \eta \frac{\rho \dot{m}_s}{\rho_{s_o}} \right) \left( \hat{C}_P - \frac{R_u}{\bar{M}} \right) \right]. \quad (7-22)$$

The solution of Eq. 7-21 is

$$T_s = C_1 + C_2 \exp(-Dx). \quad (7-23)$$

The integration constants are determined from the boundary conditions:

$$\left. \begin{aligned} T_s(0) &= \bar{T}_1 \\ T_s(1) &= \bar{T}_I \end{aligned} \right\} \quad (7-24)$$

and the final solution is

$$T_s = \frac{\bar{T}_I - \bar{T}_1 \exp(-D) + (\bar{T}_1 - \bar{T}_I) \exp(-Dx)}{1 - \exp(-D)} \quad (7-25)$$

The mass loss rates  $\dot{m}_s$  and  $\dot{m}_g$  and the char layer thickness  $\ell$  are obtained from this equation with the following equations

$$\left. \begin{aligned} \dot{m}_g / \Delta \rho &= \dot{m}_s / \rho_{s_0} \\ \left( \frac{\partial T_s}{\partial x} \right)_{x=0} &= \frac{\ell}{k_s} \left( \dot{m}_s H_C - q_{aero} \right) \\ \left( \frac{\partial T_s}{\partial x} \right)_{x=1} &= - \dot{m}_g \Delta H_P \frac{\ell}{k_s} \end{aligned} \right\} \quad (7-26)$$

where energy transfer into the uncharred layer is neglected. Thus

$$\left. \begin{aligned} \dot{m}_s &= \frac{\frac{\rho_{s_0}}{\Delta \rho} q_{aero}}{H_C + \Delta H_P + D' (\bar{T}_1 - \bar{T}_I)} \\ \dot{m}_g &= \frac{q_{aero}}{H_C + \Delta H_P + D' (\bar{T}_1 - \bar{T}_I)} \\ \ell &= \frac{k_s}{q_{aero} D'} \left[ H_C + \Delta H_P + D' (\bar{T}_1 - \bar{T}_I) \right] \ln \left[ \frac{\Delta H_P + D' (\bar{T}_1 - \bar{T}_I)}{\Delta H_P} \right] \end{aligned} \right\} \quad (7-27)$$

where

$$D' = \hat{C}_{P_s} + \left( \hat{C}_P - \frac{R_u}{\bar{M}} \right) \left( \frac{\Delta\rho + \eta\rho}{\rho_{s_0}} \right) \quad (7-28)$$

The inputs used to obtain an exact solution to a quasi-steady-state ablation problem are listed in Table 4.

Numerical solutions were obtained using the finite difference equations. The assumption of incompressibility was satisfied by specifying the pyrolysis gas density to be constant. In an attempt to satisfy the assumption of local thermal equilibrium between the pyrolysis gases and the char layer a very large value was used for the proportionality constant appearing in the equation for  $H_A$ , the convective heat transfer coefficient,

$$H_A = \frac{K_h v}{N_{Pr}} \sum_i \frac{\rho_i C_{P_i}}{M_i} . \quad (7-29)$$

Calculations were made using a value for  $K_h$  of  $5 \times 10^5$  1/m yet a temperature difference of  $1.5^\circ$  K exists between the char layer and the pyrolysis gases at the front surface. These results are compared with the exact solution in Table 5. Note that the char thickness and mass loss rates are within 2% of the exact solution.

An additional set of calculations was made in which the pyrolysis gas temperature was set equal to the char layer temperature and the term,  $H_A(T_s - T)$ , appearing in the char layer equation was replaced using the following equation

Table 4.- Inputs Used in Exact Solution to  
Quasi-Steady-State Ablation Case.

Quantity	Value
$q_{\text{aero}}$	$0.8 \times 10^5 \text{ W/m}^2$
$k_s$	$0.624 \text{ W/m}^2\text{-}^\circ\text{K}$
$\rho_{s_0}$	$320. \text{ kg/m}^3$
$\Delta\rho$	$320. \text{ kg/m}^3$
$\hat{C}_{p_s}$	$2090. \text{ J/kg-}^\circ\text{K}$
$\hat{C}_p$	$2090. \text{ J/kg-}^\circ\text{K}$
$\bar{T}_l$	$2222. \text{ }^\circ\text{K}$
$\bar{T}_I$	$556. \text{ }^\circ\text{K}$
$\Delta H_P$	$2.324 \times 10^6 \text{ J/kg}$
$H_C$	$2.324 \times 10^6 \text{ J/kg}$
$\bar{M}$	$0.029 \text{ kg/g-mole }^\circ\text{K}$

Table 5.- Comparison of the Exact Solution and the Numerical Solution Obtained with  $K_h = 5. \times 10^5$  1/m for a Quasi-Steady State Condition.

Parameter	Numerical Solution	Exact Solution	% Error
$\dot{m}_s, \text{ kg/m}^2\text{sec}$	$7.304 \times 10^{-2}$	$7.185 \times 10^{-2}$	1.66
$\dot{m}_g, \text{ kg/m}^2\text{sec}$	$7.301 \times 10^{-2}$	$7.185 \times 10^{-2}$	1.61
$\ell, \text{ m}$	$2.924 \times 10^{-3}$	$2.973 \times 10^{-3}$	-1.65

$$H_A(T_s - T) = \frac{1}{\ell} \left( \dot{m}_g - \eta \rho \dot{m}_s / \rho_{s_o} \right) \left[ \hat{C}_p - \frac{R_u}{M} \frac{\partial T_s}{\partial x} \right]. \quad (7-30)$$

Thus the assumption of local thermal equilibrium between the pyrolysis gases and the char layer was satisfied. Results from this set of calculations shown in Fig. 9 are within 1% of the exact solution. Note that the system reached a quasi-steady-state condition after only 30 sec. The near discontinuity in the surface removal rate curve illustrates the three regimes of mass removal at the surface. The initial segment of the curve represents that portion of time when oxidation of the char layer was governed by the exponential rate equation. The second portion of lesser slope represents the time period when the rate of oxidation of the char was governed by the rate of diffusion of oxygen through the boundary layer. The final portion of the curve represents the time during which the char layer was subliming.

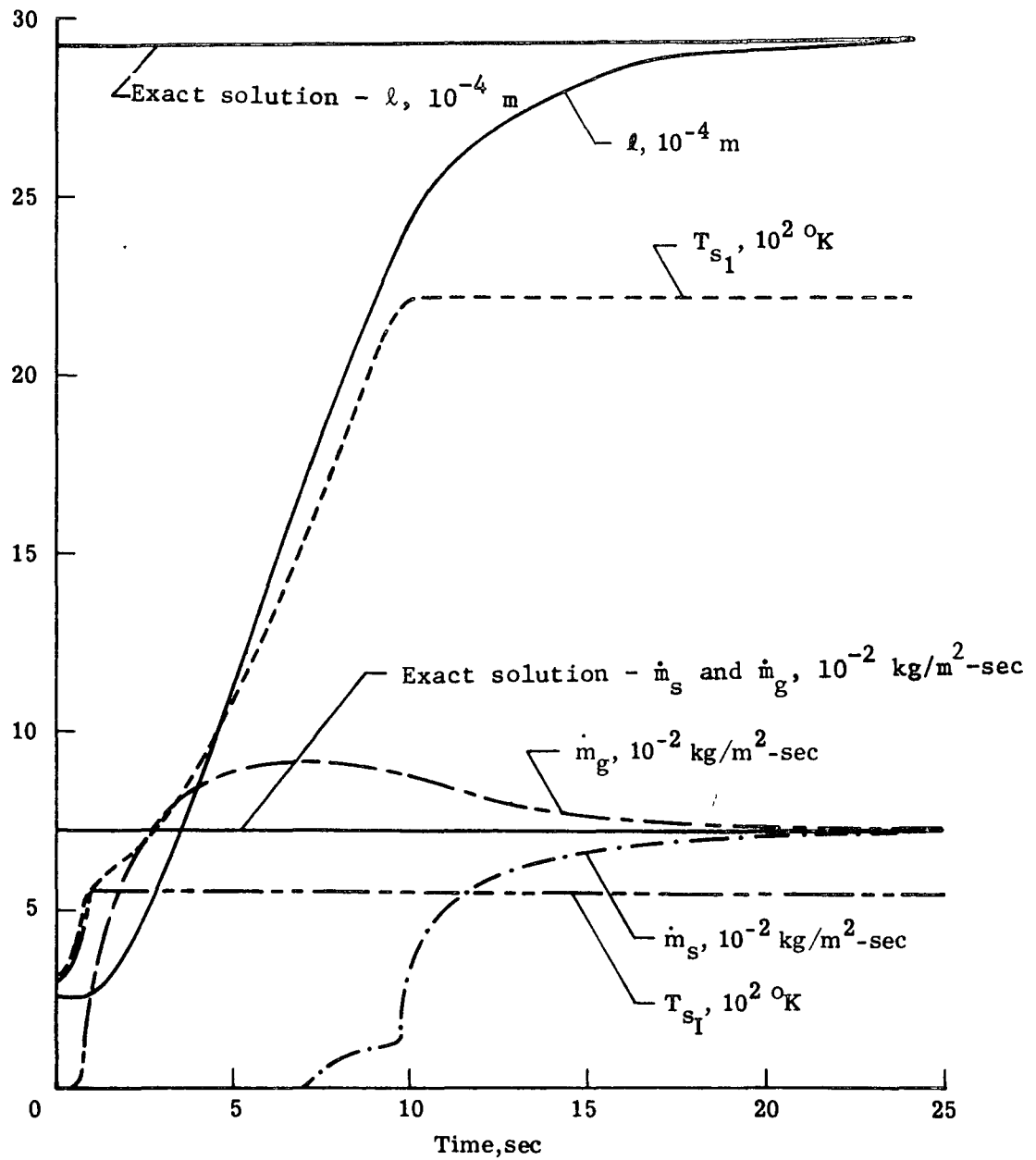


Figure 9.- Numerical results for  $\dot{m}_s$ ,  $\dot{m}_g$ ,  $\ell$ , surface temperature, and pyrolysis temperature for a case run to quasi-steady-state condition.



## CHAPTER VIII

### RESULTS AND DISCUSSION

The analysis of heat transfer and ablation mechanisms present in ablative thermal protection systems during entry is of major importance in the design of heat shields for aerospace applications. The role that ablation analysis plays in the total program of heat shield design is shown in Fig. 10. The first stage of the program involves defining the entry environment. This definition is obtained from trajectory analysis experts. Once the environment is defined a heat shield material can be selected - the material may be one of a family of existing materials or it may be necessary to develop a new material which possesses characteristics required for a particular trajectory. Thermo-physical property data are then obtained. The definition of the environment and the material characterization are then used in a computer program to determine the response of the material to entry conditions. Because of uncertainties in the material characterization and simplifying assumptions made in the analysis, it is necessary to have checks on the results. Initially, the material is subjected to simulated entry conditions in our ground test facilities. Later the material may be flight-tested. There frequently is feedback from the analysis and ground test phases to the materials development phase to obtain improved materials. It is sometimes necessary to adjust the property data which typically contains many uncertainties to obtain good agreement between numerical and experimental data. Once the

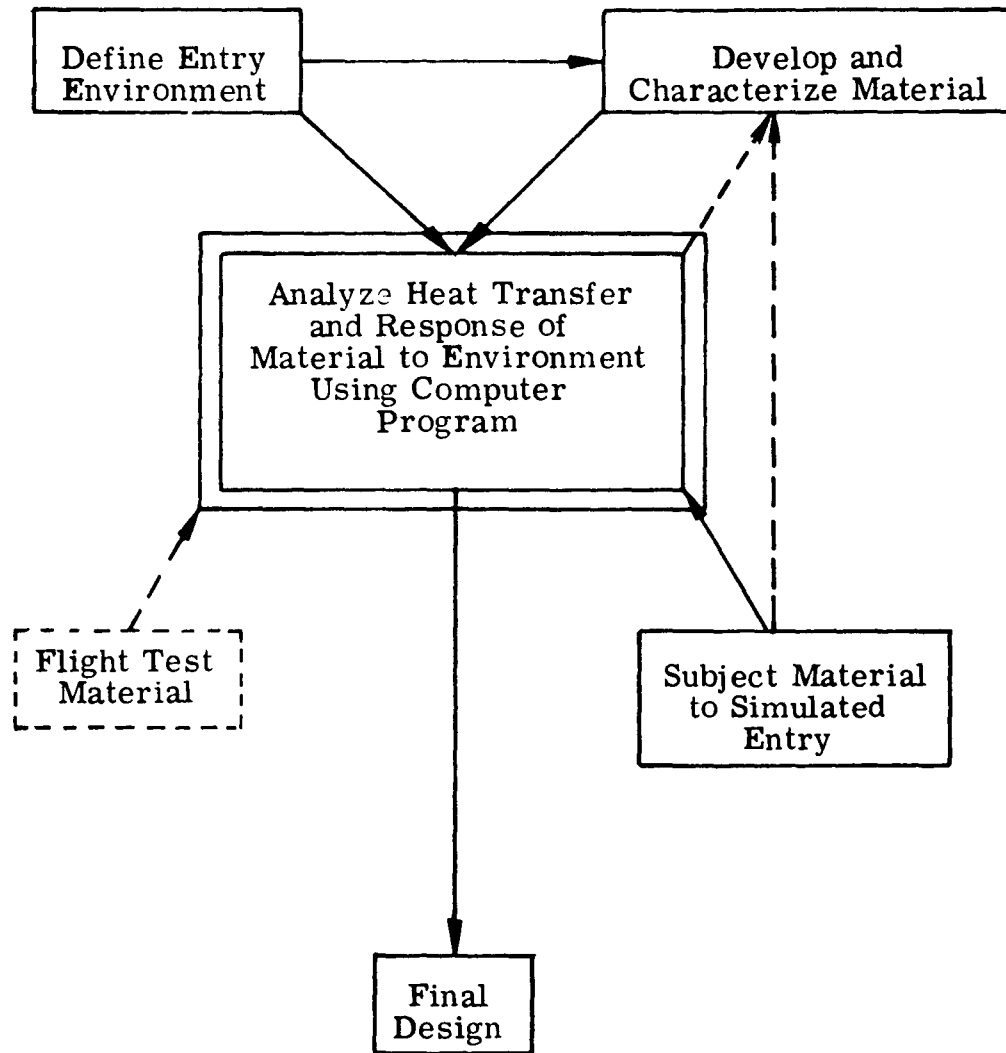


Figure 10.- The role of ablation analysis in the design of thermal protection systems for aerospace applications.

computed results are found to be satisfactory the analysis is used to determine the amount of ablation material required for the mission.

Results from a typical computer calculation for an ablation system subjected to a square heat pulse are presented in Figs. 11-13 as an illustration of the type of data available from this analysis. The heating rate, enthalpy, and pressure histories for this calculation are given in Table 6. The ablation system properties considered in this calculation are those given in Table 2. Figure 11 shows time histories of surface removal rate, pyrolysis rate, char thickness, char surface temperature, and pyrolysis gas temperature at the surface for this calculation. Of particular interest in Fig. 11 is the short time during which the mode of performance is highly transient. After 100 seconds the temperature and mass transfer rates are changing much slower than initially. The spike in  $\dot{m}_g$  occurring at 10 sec corresponds to the rapid increase in system temperature at initiation of heating. The sharp drop in  $\dot{m}_g$  results from the growth of the char layer which insulates the pyrolysis zone and the blocking effect of the pyrolysis gases which reduces the rate of heat transfer to the char surface. The substantial difference in temperature of the char and pyrolysis gases at times less than 50 sec results from two factors —1) Because of the thin char layer at early times, the fluid mechanical time is very small as is the energy transfer per mass of pyrolysis gas; and 2) For very low surface pressures, the reduction in gas temperature

Table 6.- Trajectory Data Used in Making Calculation for a Typical Ablation System.

Parameter	Value
$q_c, \text{W/m}^2$ , at	
time, sec	
0	$2.162 \times 10^3$
10	$8.0 \times 10^5$
1000	$8.0 \times 10^5$
$P_w, \text{N/m}^2$ , at	
time, sec	
0	$1.0 \times 10^{-6}$
9	$1.0 \times 10^{-4}$
29	$9.0 \times 10^{-4}$
39	$1.0 \times 10^{-1}$
1000	$1.0 \times 10^{-1}$
$H_e, \text{J/kg}$	$3.1 \times 10^5$
$C_e$	0.23

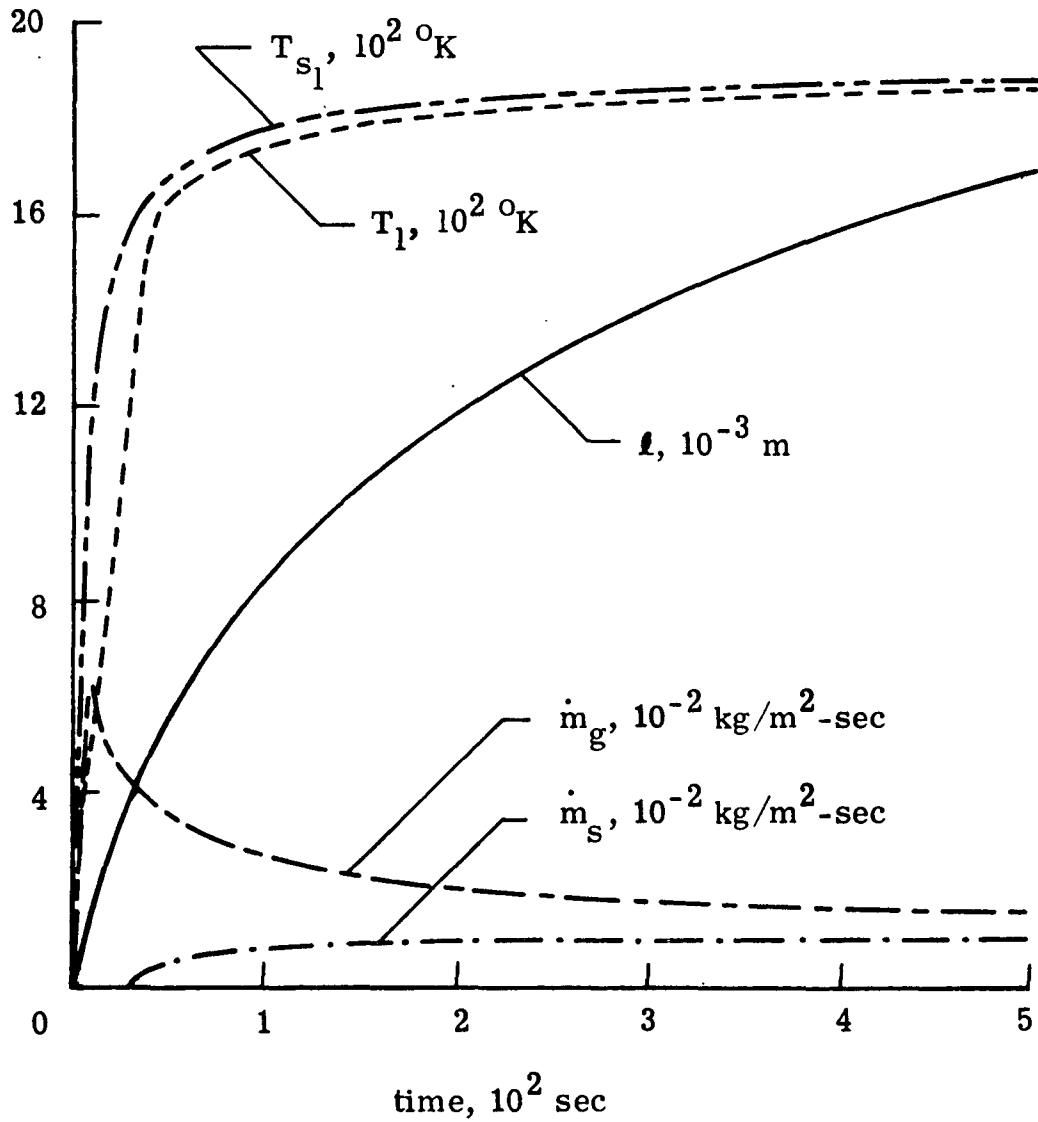


Figure 11.- Typical time histories of  $\dot{m}_s$ ,  $\dot{m}_g$ ,  $l$ , surface temperature, and pyrolysis gas temperature at the surface for an ablation system subjected to a square heat pulse.

associated with expansion of the pyrolysis gas flowing through the char layer is appreciable. The rate controlled and diffusion controlled regimes of surface oxidation are obvious in Fig. 11. The initial steep slope (highly temperature dependent) is associated with the rate controlled oxidation regime. The  $\dot{m}_s$  curve undergoes an orderly transition on the much flatter region which corresponds to the diffusion controlled oxidation regime.

Figures 12 and 13 show profiles of pyrolysis gas temperature, molecular weight, mass flow rate, and pressure and char layer temperature and porosity at times of 50 and 500 sec, respectively, for the case whose data are presented in Fig. 11. Note that  $x = 0$  is the char layer surface and  $x = 1$  is the pyrolysis zone. Of particular interest in Fig. 12 is the greater temperature difference between the char layer and pyrolysis gas near the pyrolysis zone. The difference in temperature is greater in this region because of the larger gradient in char layer temperature. As the pyrolysis gas temperature increases to about 1200° K the chemical reactions and mass transfer processes within the system become significant. The decrease in molecular weight results from a breaking down of larger molecular weight species and loss of carbon through deposition of solid carbon in the porous char layer. The rate of carbon deposition is reflected in the reduced local mass flow rate ( $\dot{m}$ ). The net carbon deposited is indicated by the porosity profile.

The profiles in Fig. 13 are of the same form as those in Fig. 12. Because of the larger char layer thickness at 500 sec the pyrolysis gas temperature is nearer the char layer temperature in the region near the surface.

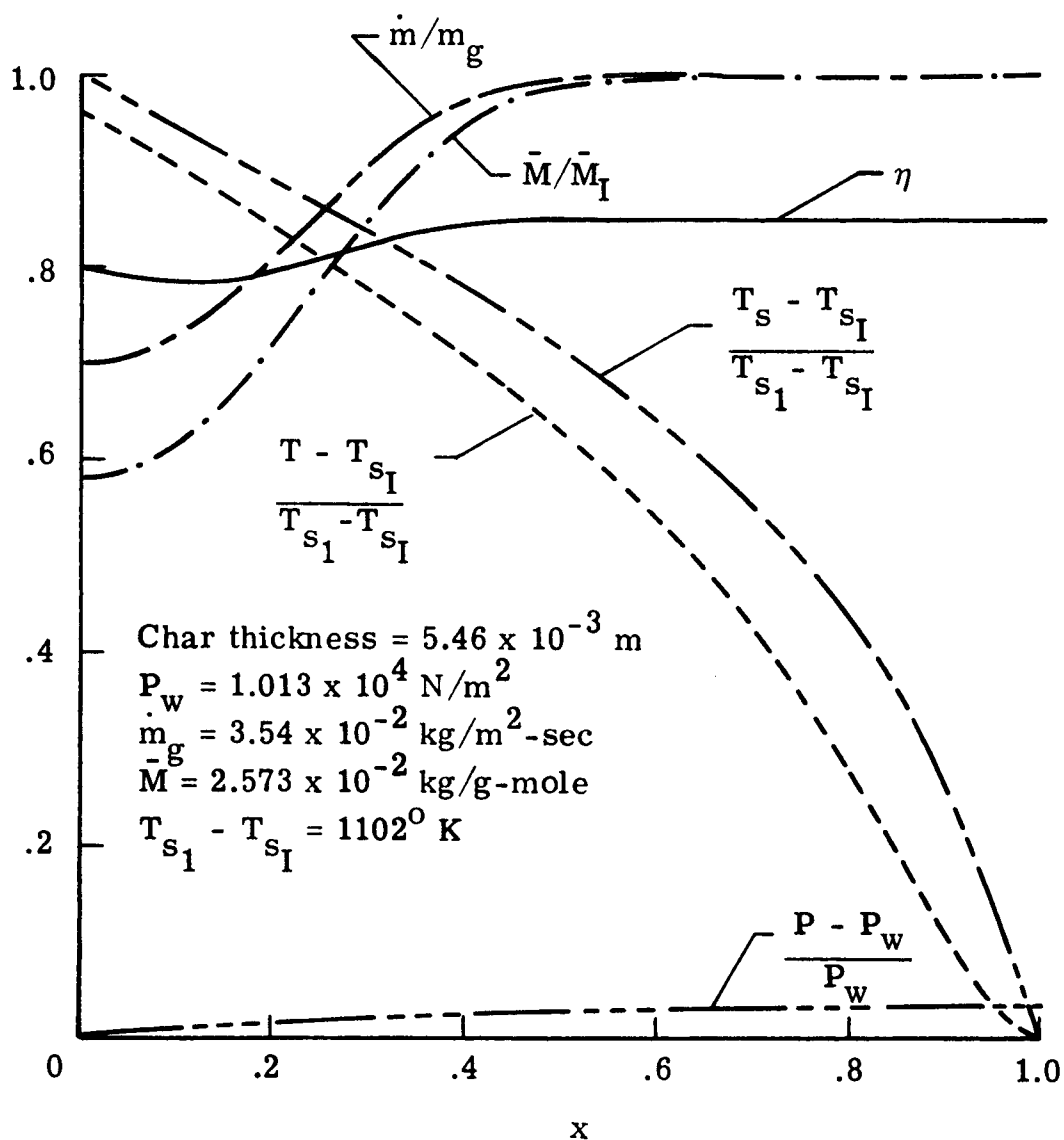


Figure 12.- Profiles of pyrolysis gas temperature, char layer temperature, pyrolysis gas molecular weight, char porosity, local mass flow rate, and pyrolysis gas pressure at a time of 50 sec for the case represented in Fig. 11.

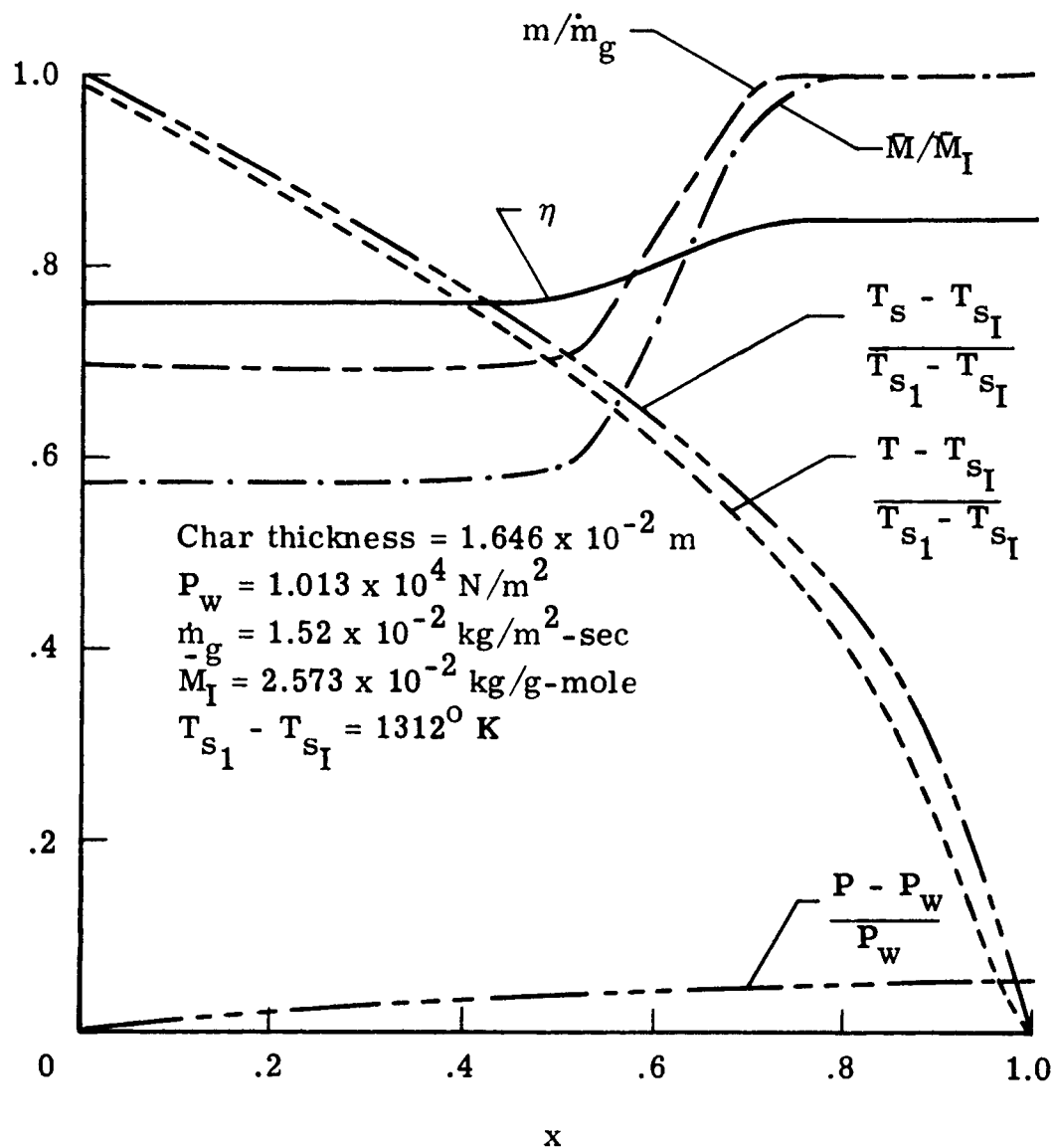


Figure 13.- Profiles of pyrolysis gas temperature, char layer temperature, pyrolysis gas molecular weight, char porosity, local mass flow rate, and pyrolysis gas pressure at a time of 500 sec for the case represented in Fig. 11.



## CHAPTER IX

### SUMMARY

The differential equations governing the transient response of a one-dimensional ablative thermal protection system undergoing stagnation ablation have been derived for the general case of thermal non-equilibrium between the pyrolysis gases and the char layer and kinetically controlled chemical reactions and mass transfer between the pyrolysis gases and the char layer. The boundary conditions have been written for the particular case of stagnation heating with surface removal by oxidation or sublimation and pyrolysis of the uncharred layer occurring in a plane.

The governing equations and boundary conditions have been solved numerically using the modified implicit method (Crank-Nicolson method). Exact solutions were obtained for a number of simplified problems. Numerical results compared favorably with exact results in every instance.

Numerical results were presented for a typical ablation system subjected to a square heat pulse. The effects of chemical reactions and mass transfer are pronounced.

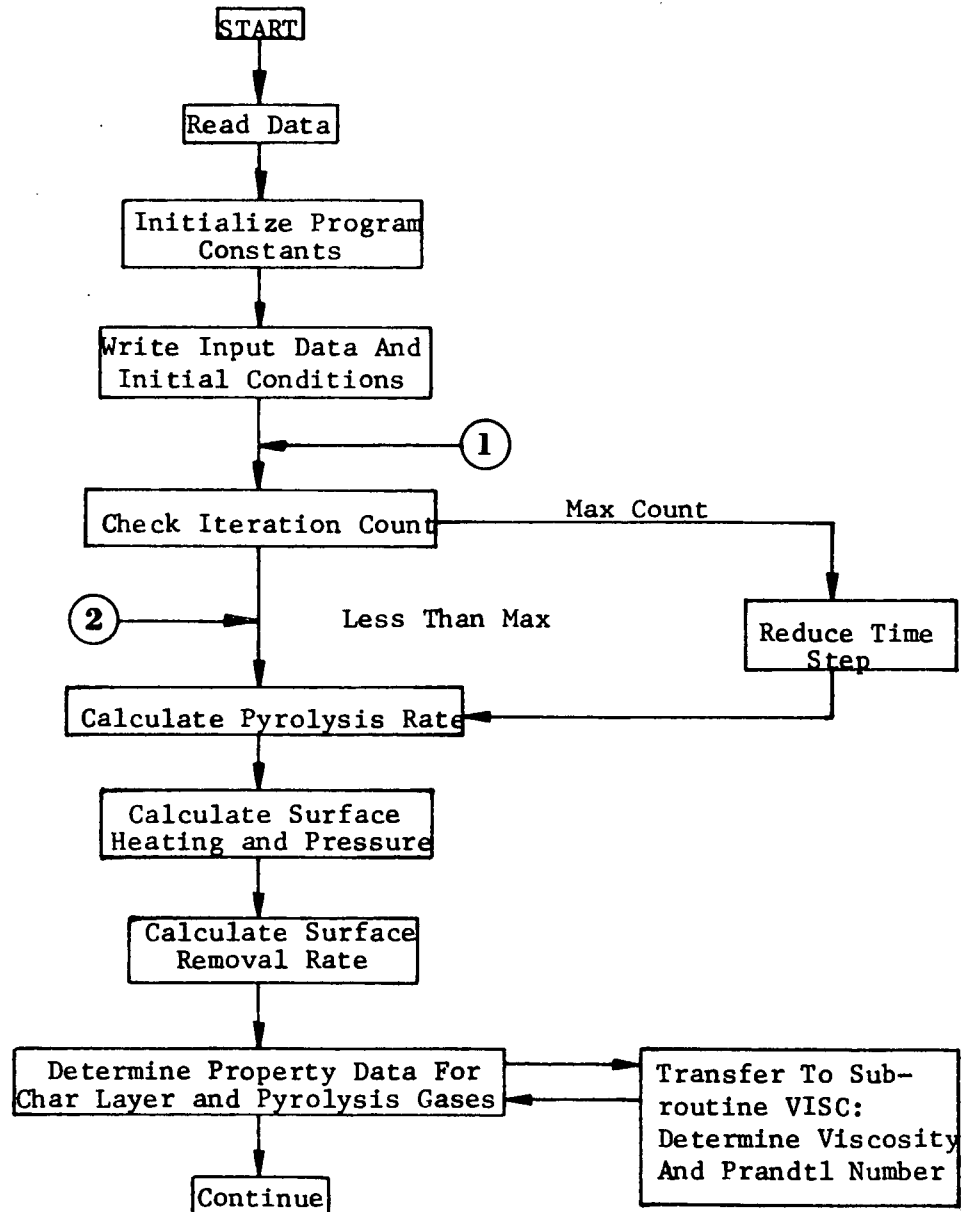
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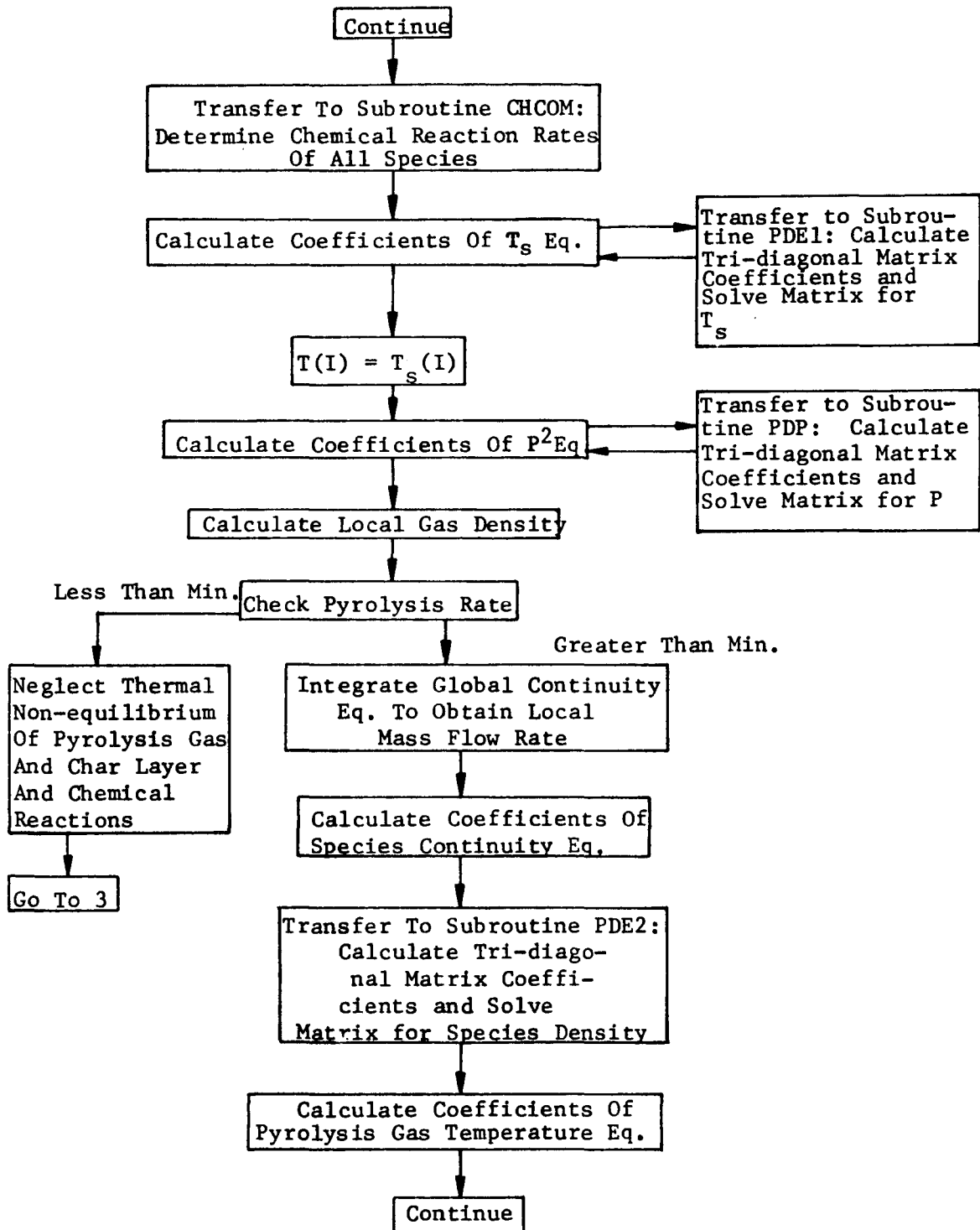
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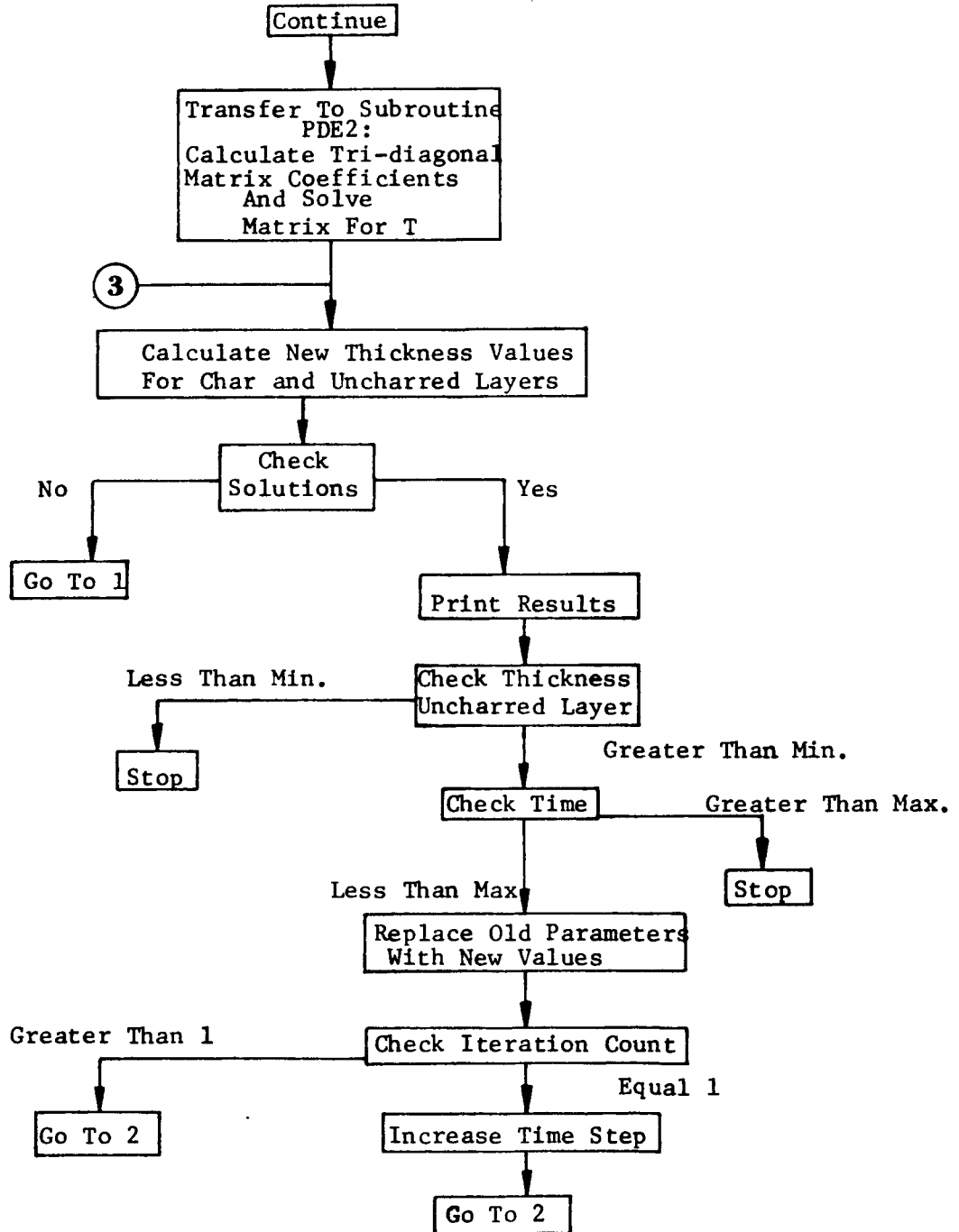
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APPENDIX A  
GENERAL FLOW CHART







## APPENDIX B

### PROGRAM USAGE INSTRUCTIONS

This program calculates the transient response of a one-dimensional ablative thermal protection system subjected to stagnation heating. It treats thermal non-equilibrium between the pyrolysis gases and the char layer, mass transfer between the fluid and solid phases, and a total of nine chemical reactions involving twelve gaseous species plus solid carbon. Surface removal by oxidation or sublimation and pyrolysis of the uncharred material occurring in a plane are considered. It considers a single layer of ablation material backed up by a single layer of insulation material with heat sinks between the ablation material and the insulation and behind the insulation. A maximum of 50 stations each may be considered for the char layer and the uncharred layer of the ablation material and a maximum of 10 stations may be considered for the insulation.

### INPUT

FORTRAN IV NAMELIST with the names PERM, PIKUP, and LIST is used to load the input data. PERM contains physical constants, program constants and tables of thermodynamic and chemical kinetics data which are considered to be permanent inputs. PIKUP contains initial solutions plus selected program constants and material properties. These data are changed when beginning a computer calculation at some time other



than 0. seconds. LIST contains those data and system parameters which are most frequently changed from one calculation to another. The following list contains the input variables with the dimensions used in the program. The NAMELIST name containing each variable is indicated in its description. The size of an array is limited to the dimensions stated.

FORTRAN VARIABLE	DESCRIPTION
AC	Specific reaction rate constant for first order oxidation of char layer (LIST).
ACEF(12)	Specific reaction rate constant for forward chemical reaction (PERM).
ACER(12)	Specific reaction rate constant for reverse chemical reaction (PERM).
AEXP	Specific reaction rate constant for pyrolysis of uncharred material (LIST).
ALFC	Weight factor for transpiration effectiveness of mass removal by oxidation or sublimation (LIST).
ALFP	Weight factor for transpiration effectiveness of pyrolysis gases (LIST).
ALPHA	Absorptivity of char surface (LIST).
BC	Activation temperature for first order oxidation of char layer (LIST).
BCEF(12)	Activation temperature for forward chemical reaction (PERM).
BCER(12)	Activation temperature for reverse chemical reaction (PERM).
BEXP	Activation temperature for pyrolysis of uncharred material (LIST).
CE	Mass fraction of oxygen at edge of boundary layer (LIST).

CPKT(40,12)	Table of gaseous species heat capacity versus temperature (PERM).
CPPPV	Constant heat capacity of insulation layer (LIST).
CPPT(40)	Table of uncharred material heat capacity versus temperature (LIST).
CPSV	Constant heat capacity of char layer (LIST).
CRNI	Crank-Nicolson factor, $1/2$ for modified implicit solutions (PERM).
DHC	Heat of combustion of char layer (LIST).
DHP	Heat of pyrolysis of uncharred material (LIST).
DIFER	Convergence criteria for solid temperature equation (PERM).
DRHO	Difference in density of uncharred material and density of char layer at the pyrolysis zone (LIST).
DT	Time increment (PIKUP).
DX	Distance between finite difference stations in char layer in region of course grid spacing (PERM).
DX1	Distance between finite difference stations in char layer in region of fine grid spacing (PERM).
DXP	Distance between finite difference stations in uncharred layer in region of course grid spacing (PERM).
DXP1	Distance between finite difference stations in uncharred layer in region of fine grid spacing (PERM).
DXPP	Distance between finite difference stations in insulation layer (PERM).
EPSP	Emissivity of radiating heat sink surface behind insulation layer (LIST).
EPSS	Emissivity of char surface (LIST).
ETA(50)	Porosity of char layer (PIKUP).
HC	Heat of sublimation of char layer (LIST).
HE	Enthalpy of free stream (LIST).

HKT(40,13)	Table of gaseous species enthalpy versus temperature (PERM).
HSTT(40)	Table of char layer enthalpy versus temperature (PERM).
HTSK	Value of $\rho \hat{C}_p l$ for heat sink at uncharred layer insulation layer interface (LIST).
HTSKP	Value of $\rho \hat{C}_p l$ for heat sink behind insulation layer (LIST).
I	Number of finite difference stations in char layer (PERM).
IL	Thickness of insulation layer (LIST).
IOPTI	Trigger for selecting method of computing pyrolysis rate (LIST).
IOPTP	Trigger for selecting method of determining wall pressure (LIST).
IOPT1	Trigger for selecting method of computing surface removal by sublimation (LIST).
IZ	Total number of finite difference stations in char layer, uncharred layer and insulation layer (PERM).
ITR	Maximum iteration count (LIST).
JK	Number of finite difference stations in uncharred layer (PERM).
KPPI	Thermal conductivity of uncharred layer at pyrolysis zone (PIKUP).
KPPV	Constant thermal conductivity of insulation layer (LIST).
KPT(40)	Table of uncharred material thermal conductivity versus temperature (LIST).
KSPI	Thermal conductivity of char layer at pyrolysis zone (PIKUP).
KSPl	Thermal conductivity of char layer at surface (PIKUP).
KST(40)	Table of char layer thermal conductivity versus temperature (LIST).
KT	Number of gaseous species considered (PERM).
KUPT(40,12)	Table of gaseous species thermal conductivity versus temperature (PERM).

L	Initial thickness of char layer (PIKUP).
LAM	Ratio of mass char layer removed to free stream oxygen consumed in first order oxidation of char (LIST).
LP	Initial thickness of uncharred layer (PIKUP).
LPMIN	Minimum thickness of uncharred layer (PERM).
M(13)	Molecular weight of chemical species (PERM).
MCPP	Order of interpolation in CPPT (LIST).
MFK(50,12)	Initial mole fraction of gaseous species (PIKUP).
MFKI(12)	Mole fraction of gaseous species at pyrolysis zone (LIST).
MGDOT	Initial rate of pyrolysis of uncharred layer (PIKUP).
MKP	Order of interpolation in KPT (LIST).
MKS	Order of interpolation in KST (LIST).
MNO	Order of interpolation in HSTT, HKT, CPKT, MUKT and KUPT (PERM).
MQC	Order of interpolation in QCTAB (LIST).
MSDOT	Initial rate of surface removal (PIKUP).
MSQPT	Order of interpolation in SQPT (LIST).
MUKT(40,12)	Table of gaseous species viscosity versus temperature (PERM).
NCPP	Number of entries in KPT (LIST).
NKS	Number of entries in KST (LIST).
NNO	Number of entries in HSTT, HKT, CPKT, MUKT and KUPT (PERM).
NQC	Number of entries in QCTAB (LIST).
NRCT	Number of chemical reactions considered (PERM).
NSQPT	Number of entries in SQPT (LIST).
P	Initial pyrolysis gas pressure (PIKUP).

PMV	Constant permeability of char layer (LIST).
PRNTFRQ	Time interval for printing output (PIKUP).
PROPC	Proportionality constant in expression for $H_A$ (LIST).
PTIME	Time at start of calculation (PIKUP).
QCTAB(40)	Table of cold wall heating rate versus time (LIST).
QRS	Radiant heat transfer at surface (LIST).
RAD	Vehicle nose radius for hypersonic velocities (LIST).
RHOPPV	Constant density of insulation layer (LIST).
RHOST	Theoretical density of char layer (LIST).
RU	Universal gas constant (PERM).
SGMA	Stephan-Boltzman constant (PERM).
SQPT(40)	Table of square root of wall pressure versus time (LIST).
T	Initial pyrolysis gas temperature (PIKUP).
T1BAR	Sublimation temperature of char layer (LIST).
TCPP(40)	Temperature table for CPPT (LIST).
TEMP (40)	Temperature table for HSTT, HKT, CPKT, MUKT and KUPT (PERM).
TIBAR	Maximum temperature of pyrolysis zone (LIST).
TIME	Time at start of calculation (PIKUP).
TIMET(40)	Time table for QCTAB(LIST).
TKP(40)	Temperature table for KPT (LIST).
TKS(40)	Temperature table for KST (LIST).
TMPRESS(40)	Time table for SQPT (LIST).
TRAB	Trigger for selecting blocking approximation (LIST).
TREF	Transpiration effectiveness (LIST).
TS	Initial char layer temperature (PIKUP).

## OUTPUT

The computed results are available in tabular form. The following tabular data are printed at time intervals determined by the input PRNTFRQ.

1. Time, sec.
2. Current time increment, sec.
3. Number of iterations required to obtain solution.
4. Temperature of char layer surface, K.
5. Temperature of pyrolysis gases leaving char layer, K.
6. Ratio of energy conducted into char layer to cold wall heating rate.
7. Surface removal rate,  $\text{kg/m}^2\text{-sec.}$
8. Rate of pyrolysis of uncharred layer,  $\text{kg/m}^2\text{-sec.}$
9. Pyrolysis gas mass injection rate at surface,  $\text{kg/m}^2\text{-sec.}$
10. Char layer thickness, m.
11. Uncharred layer thickness, m.
12. Temperature at each station of char layer, uncharred layer and insulation layer, K.
13. Porosity of char layer at each station.
14. Pyrolysis gas temperature at each station, K.
15. Pyrolysis gas pressure at each station,  $\text{N/m}^2$ .
16. Mole fraction of gaseous species at each station.
17. Average molecular weight of pyrolysis gas at each station, kg/m-mole.
18. Mass flow rate of pyrolysis gases at each station,  $\text{kg/m}^2\text{-sec.}$

## APPENDIX C

### PROGRAM IN FORTRAN 600 STATEMENTS

PROGRAM ABLATE(INPUT,OUTPUT,TAPE5=INPUT,TAPE2=OUTPUT)

A NUMERICAL SOLUTION OF THE DIFFERENTIAL EQUATIONS GOVERNING THE  
TRANSIENT RESPONSE OF A ONE-DIMENSIONAL ABLATION SYSTEM INCLUDING  
EFFECTS OF THERMAL NON-EQUILIBRIUM, MASS TRANSFER, AND CHEMICAL  
REACTIONS.

REFERENCE-- CLARK, RONALD K.- A NUMERICAL ANALYSIS OF THE TRAN-  
SIENT RESPONSE OF AN ABLATION SYSTEM INCLUDING EFFECTS OF THER-  
MAL NON-EQUILIBRIUM, MASS TRANSFER, AND CHEMICAL KINETICS.  
DOCTOR OF PHILOSOPHY DISSERTATION, VIRGINIA POLYTECHNIC IN-  
STITUTE AND STATE UNIVERSITY, BLACKSBURG, VA. 1972.

# PRIMARY INPUTS

DHC	HEAT OF COMBUSTION OF CHAR LAYER	A	15
DHP	HEAT OF PYROLYSIS	A	16
DRHO	DENSITY CHANGE ACROSS PYROLYSIS INTERFACE	A	17
DT	TIME INCREMENT	A	18
EPSP	BACK SURFACE EMISSIVITY	A	19
EPSS	CHAR SURFACE EMISSIVITY	A	20
HC	HEAT OF SUBLIMATION OF CHAR LAYER	A	21
HE	ENTHALPY OF FREE STREAM	A	22
HTSK	VALUE OF THERMAL CAPACITY OF HEAT SINK AT BACK OF UNCHARRED MATERIAL	A	23 24
HTSKP	VALUE OF THERMAL CAPACITY OF HEAT SINK AT BACK OF INSULATION LAYER	A	25 26
IOPTI	TRIGGER FOR SELECTING METHOD OF COMPUTING PYROLYSIS RATE. (IOPTI=0 NO RESTRICTION ON TEMPERATURE OF PY- ROLYSIS ZONE- PYROLYSIS RATE COMPUTED USING ARR- HENIUS TYPE RATE EQUATION, IOPTI=1 TEMPERATURE OF PYROLYSIS ZONE LIMITED TO TIBAR- PYROLYSIS RATE COM- PUTED USING ENERGY BALANCE WHEN TS(I)=TIBAR)	A	27 28 29 30 31 32
IOPT1	TRIGGER FOR SELECTING MODE OF BEHAVIOR OF SURFACE TEMPERATURE DURING SUBLIMATION. (IOPT1=0 NO RE- STRICTION ON SURFACE TEMPERATURE, IOPT1=1 SURFACE TEMPERATURE LIMITED TO TIBAR)	A	33 34 35 36



C	IOPTP	TRIGGER FOR SELECTING METHOD OF COMPUTING WALL PRES-	A	37
C		SURE. (IOPTP=1 USE TABLE LOOKUP, IOPTP=0 COMPUTE	A	38
C		WALL PRESSURE FROM HYPERSONIC FLOW THEORY)	A	39
C	KT	NUMBER OF GASEOUS SPECIES CONSIDERED	A	40
C	LOP	INITIAL THICKNESS OF UNCHARRED LAYER	A	41
C	NRCT	NUMBER OF CHEMICAL REACTIONS CONSIDERED	A	42
C	QCTAB	TABLE OF COLD WALL CONVECTIVE HEATING RATE VS TIME	A	43
C	QRS	RADIANT HEATING RATE	A	44
C	RAD	RADIUS OF BODY	A	45
C	RHOST	THEORETICAL DENSITY OF CHAR MATERIAL	A	46
C	SQPT	TABLE OF WALL PRESSURE VS TIME	A	47
C	TIBAR	MAXIMUM TEMPERATURE OF PYROLYSIS ZONE USED WITH	A	48
C	TIBAR	SUBLIMATION TEMPERATURE OF CHAR LAYER	A	49
C			A	50
C	CHEMICAL SPECIES IDENTIFICATION-		A	51
C	1. CH4	2. H2	3. C2H4	A 52
C	4. C2H2	5. CO	6. H2O	A 53
C	7. NH3	8. N2	9. CO2	A 54
C	10. HCN	11. C2H6	12. C6H6	A 55
C	13. C (SOLID)			A 56
C				A 57
C	FOR DOUBLE SUBSCRIPTED QUANTITIES- FIRST SUBSCRIPT REFERS TO		A	58
C	REACTION, STATION, OR TEMPERATURE AND SECOND SUBSCRIPT REFERS		A	59
C	TO CHEMICAL SPECIES.		A	60
C			A	61
C			A	62
C	DIMENSION ALPHA1(110), ALPHA2(110), ALPHA3(110), ALPHA4(110), ARH(		A	63
C	150), ALPHB3(110), ALPHB4(110), ALPHP1(110), ALPHP2(110), ALPHP3(11		A	64
C	20), ALPHP4(110), BETA1(50), BETA2(50), BETA3(50), YP(50), BRH(50),		A	65
C	3 BETB3(50), BETP1(50), BETP2(50), BETP3(50), CPK(50,12), BET32(50)		A	66
C	4, CPKT(40,12), CPKTV(40), CPP(100), CPPT(40), CPS(50), AL1(50), DE		A	67
C	5B2(50,12), DEB3(50), DEL1(50,12), DEL2(50,12), DEL3(50), DEP1(50,1		A	68
C	62), DEP2(50,12), DEP3(50), DETADX(50), AB2(50), ROM(50), DKPDX(10		A	69
C	70), DKSDX(50), DVDX(50), AB3(50), TP(50), HA(50), PAMGDOT(50,12),		A	70
C	8EPSB3(50), HK(50,13), HKT(40,13), HKT(40), HRSUM(50), HS(50), HST		A	71

9(50), APL(50), HSTT(40), KG(50), KP(100), KPT(40), KS(50), P(50),	A	72
\$TIMET(40), QCTAB(40), TMPRES(40), SQPT(40), TCPP(40), TKP(40), EPS	A	73
\$P1(50), RHOP(100), RM(50), ROM(50), TS(110), EPSA1(50), EPSA2(50),	A	74
\$ TSP(110), V(50), MFKI(12), EPSA3(50), EPSP2(50), EPSP3(50), EPSB2	A	75
\$(50), PROM(50), AMDOT(50), AP(50), KPP(110), CPPP(110), RHOPP(110)	A	76
\$, DRODX(50), YETA(50), NRHOK(12), AT(50), ATS(110), YTS(110), YT(5	A	77
\$0), YRHO(50), YRHOK(50,12), TKS(40), KST(40), PTS(110), PT(50), VC	A	78
\$(50), DMBROX(50), DTDX(50), AINT1(50), AINT3(50), SPECIES(13)	A	79
COMMON ACEF(12),ACER(12),BCEF(12),BCER(12),CRNI,KUPT(40,12),<JPTV(	A	80
140),M(13),MFK(50,12),MNO,NNO,MU(50),MUKT(40,12),MUKTV(40),PR(50),R	A	81
2(50,12),RHO(50),RHOK(50,12),RHOKP(50,12),T(50),TEMP(40),NRCT,<T,RU	A	82
3,NSTEP,RJCPM(50),RS(50),RHR(50,12),RAS(50),DHK(50,12),DHJ(50,12),H	A	83
4RJSUM(50)	A	84
COMMON /PDE1/ ALPHI1,ALPHI2,ALPHI3,ALPHI4,ALPHIP1,ALPHIP2,ALPHIP3,	A	85
1ALPHIP4,GAMMI1,GAMMI2,GAMMI4,GAMMIP1,GAMMIP2,GAMMIP3,GAMMIP4,SGMA,	A	86
2DX,ALPHA1,ALPHA2,ALPHP1,ALPHP2,ALPHB3,ALPHB4,DT,L,Q,<S,LP,QPT,KSP1	A	87
3,TSP,DXP,IP,I,IO,IN,IOI,KP,LPP,LPPP,KSPI,KPPI,MGDOT,DHP,MGDOTP,QNE	A	88
4T,QPNET,KPPIP,GAMMI3,IM,EPSS,EPSP,DX1,DXP1,ALPHA4,ALPHP3,ALPHP4,AL	A	89
5PHA3,HTSK,HTSKP,IOPT1,IOPTI,T1BAR,TI3AR	A	90
COMMON /PDP/ PAL1(50),PAL2(50),PAL3(50),PAL4(50),PAP1(50),PAP2(50)	A	91
1,PAP3(50),PAP4(50),PAB3(50),PAB4(50),PWP,PP(50),PM(50),PMU,PPM,PRH	A	92
20(50),ETA(50),ETAP(50),AVGMF(50),AVGMFP(50)	A	93
COMMON /TS/ IPL,IZ1,KPP,GAMIP1,GAMIP2,GAMIP3,GAMIP4,GAMIPP1,GAMIPP	A	94
12,GAMIPP3,GAMIPP4,KAPIP1,KAPIP2,KAPIP3,KAPIP4,KAPIPP1,KAPIPP2,IL,K	A	95
2APIPP3,KAPIPP4,DXPP,KPPP1P,KPPP1Z,IZ	A	96
EQUIVALENCE (EPSA2,EPSB2,EPSP2), (AB3,DEB3)	A	97
REAL KS,MU,MUK,<PPV,KP,M,L,LP,MS,MSDOT,MGDOT,MPDOT,KST,KPT,KUPT,MU	A	98
1KTV,MUKT,KUPTV,KG,LAM,KA,LPP,MFKI,LPPP,MFK,MGDOTP,KPPI,KSPI,KSP1,K	A	99
2PPIP,IL,KPP,KPPP1Z,KPPP1P,KAPIP1,KAPIP2,KAPIP3,KAPIP4,KAPIPP1,KAPI	A	100
3PP2,KAPIPP3,KAPIPP4,LPMIN,MSDOTP	A	101
NAMelist /PERM/ SGMA,I,JK,CRNI,KT,RU,M,ACEF,BCEF,NRCT,ACER,BCER,DX	A	102
11,DX,DXP,DXPP,IZ,DIFER,DXP1,LPMIN,TEMP,MNO,NNO,HSTT,CPKT,HKT,KUPT,	A	103
2MUKT,SPECIES	A	104
NAMelist /PIKUP/ TS,P,T,ETA,MGDOT,MSDOT,MFK,L,LP,TIME,PTIME,DT,KSP	A	105

	11,KSPI,KPPI,PRNTRFQ	A 106
	NAMELIST /LIST/ PROPC,ALFC,ALFP,ALPHA,DHC,ITR,QRS,EPSS,EPSP,HC,RHO	A 107
	1ST,RAD,TIBAR,DHP,LAM,CE,AC,BC,HE,TREF,TRAB,MFKI,AEXP,BEXP,IL,CPPPV	A 108
	2,KPPV,RHOPPV,HTSK,HTSKP,CPSV,PMV,KPT,TKP,MKS,NKS,KST,CPPT,TCPP,MCP	A 109
	3P,NCPP,MKP,TIMET,QCTAB,MQC,NQC,TMPRES,SQPT,MSQPT,NSQPT,TKS,NKP,IOP	A 110
	4T1,IOPT1,TIBAR,IOTPT,DRHO	A 111
C	READ INPUT DATA	A 112
	READ (5,PERM)	A 113
	READ (5,PIKUP)	A 114
	READ (5,LIST)	A 115
C	INITIALIZE PROGRAM CONSTANTS	A 116
	KTT=KT+1	A 117
	KM=KT-2	A 118
	IM=I-1	A 119
	IN=I+1	A 120
	IN2=I+2	A 121
	IP=I+JK	A 122
	I01=IP-1	A 123
	I0=IP-2	A 124
	NITC=0	A 125
	NITA=0	A 126
	MS=M(13)	A 127
	AIN1(I)=0.	A 128
	AIN3(I)=0.	A 129
	IP1=IP+1	A 130
	IZ1=IZ-1	A 131
	NIT=0	A 132
	NITG=0	A 133
	ICHCOM=0	A 134
	NTIME=0	A 135
C	CONVERT INPUT DATA TO PROPER UNITS (SYSTEM INTERNATIONAL)	A 136
C	DATA FOR HEAT CAPACITY OF CHAR LAYER- SOLID CARBON- ARE INPUT	A 137
C	IN UNITS OF JOULES/KILOGRAM (.012 KILOGRAM/G-MOLE)	A 138
C	DATA FOR HEAT CAPACITY AND ENTHALPY ARE INPUT WITH ENERGY IN	A 139
C	UNITS OF THERMOCHEMICAL CALORIE (4.184 J/CAL)	A 140
C	DATA FOR VISCOSITY OF GASEOUS SPECIES ARE INPUT IN UNITS OF	A 141

C	POISES (0.0000001 NEWTON-SECOND/METER SQ PER POISE)	A 142
	CPSV=.012*CPSV	A 143
	DO 1 K=1,NRCT	A 144
	BCEF(K)=4.184*BCEF(K)	A 145
	ACER(K)=0.	A 146
1	BCER(K)=4.184*BCER(K)	A 147
	DO 2 N=1,NNO	A 148
	HSTT(N)=HSTT(N)*4.184	A 149
	DO 2 K=1,KT	A 150
	MUKT(N,K)=MUKT(N,K)*1.E-7	A 151
	KUPT(N,K)=KUPT(N,K)*4.184E-4	A 152
	IF (K.GT.KM) GO TO 2	A 153
	CPKT(N,K)=4.184*CPKT(N,K)	A 154
	HKT(N,K)=4.184*HKT(N,K)	A 155
2	CONTINUE	A 156
	DO 3 N=1,NNO	A 157
C	WRITE INPUT DATA	A 159
3	HKT(N,13)=4.184*HKT(N,13)	A 158
	WRITE (2,PERM)	A 160
	WRITE (2,PIKUP)	A 161
	WRITE (2,LIST)	A 162
C	INITIALIZE ALL PARAMETERS	A 163
	KS(1)=KSP1	A 164
	KS(I)=KSPI	A 165
	KP(1)=KSPI	A 166
	MGDOTP=MGDOT	A 167
	MSDOTP=MSDOT	A 168
	LPP=L	A 169
	LPPP=LP	A 170
	QPNET=SGMA*EPSP*TS(IZ)**4	A 171
	DO 6 N=1,I	A 172
	DETADX(N)=0.	A 173
	DRODX(N)=0.	A 174
	AMDOT(N)=MGDOT	A 175
	PP(N)=P(N)	A 176

	RHU(N)=0.	A 177
	RHS(N)=0.	A 178
	RS(N)=0.	A 179
	ROM(N)=0.	A 180
	DO 4 KI=1,<T	A 181
	RHOK(N,KI)=P(V)*M(KI)*MFK(N,KI)/(RU*T(N))	A 182
	ROM(N)=ROM(N)+RHOK(N,KI)/M(KI)	A 183
	RHOKP(N,KI)=RHOK(N,KI)	A 184
	DHJ(N,KI)=0.	A 185
	R(N,KI)=0.	A 186
	RHR(N,KI)=0.	A 187
4	RHO(N)=RHO(N)+RHOK(N,KI)	A 188
	PROM(N)=ROM(N)	A 189
	V(N)=-MGDUTP/(RHO(N)*ETA(N))	A 190
	KOCPM(N)=P(N)*200./(RU*T(N))	A 191
	DO 5 K=1,KT	A 192
5	PAMGDOT(N,K)=-RHOK(N,K)*V(N)	A 193
	DVDX(N)=0.	A 194
6	PRHO(N)=RHO(N)	A 195
	DO 7 N=1,IP	A 196
	TSP(N)=TS(N)	A 197
	PTS(N)=300.	A 198
	IF (N.GT.I) GO TO 7	A 199
	PT(N)=300.	A 200
	AP(N)=0.	A 201
	TP(N)=T(N)	A 202
	ETAP(N)=.85	A 203
7	CONTINUE	A 204
	DO 8 N=IP,IZ	A 205
	PTS(N)=300.	A 206
	TSP(N)=TS(N)	A 207
8	CONTINUE	A 208
	QCT=SGMA*EPSS*TS(1)**4+KS(1)*(11.*TS(1)-18.*TS(2)+9.*TS(3)-2.*TS(4	A 209
	1))/ (6.*DX1*L)	A 210
	QPT=SGMA*EPSS*TS(1)**4+KS(1)*(11.*TS(1)-18.*TS(2)+9.*TS(3)-2.*TS(4	A 211

	1)))/(6.*DX1*L)	A 212
	GO TO 12	A 213
C	BEGIN ITERATION	A 214
9	CONTINUE	A 215
	IF (NITG.EQ.0) GO TO 12	A 216
C	ESTIMATE SOLUTION AT NEXT TIME STEP	A 217
	DO 11 N=1,IZ	A 218
	TS(N)=TS(N)+YTS(N)*DT	A 219
	IF (N.GT.1) GO TO 11	A 220
	RHU(N)=RHU(N)+YRHC(N)*DT	A 221
	T(N)=T(N)+YT(N)*DT	A 222
	P(N)=P(N)+YP(N)*DT	A 223
	ETA(N)=ETA(N)+YETA(N)*DT	A 224
	DO 10 K=1,KT	A 225
10	RHOK(N,K)=RHOK(N,K)+YRHOK(N,K)*DT	A 226
11	CONTINUE	A 227
12	NIT=NIT+1	A 228
	RHOS0=RHO0*(1.-ETA(1))	A 229
C	DETERMINE HEATING AT BACK SURFACE	A 230
	QNET=SGMA*EPS*TS(IZ)**4	A 231
C	CHECK ITERATION COUNT- REDUCE TIME STEP IF MAX ITER EXCEEDED	A 232
	IF (NIT.LT.ITR) GO TO 15	A 233
	TIME=TIME-DT	A 234
	MGDOT=MGDUTP	A 235
	DO 14 N=1,IZ	A 236
	IF (N.GT.1) GO TO 14	A 237
	DO 13 K=1,KT	A 238
13	RHOK(N,K)=RHOKP(N,K)	A 239
	T(N)=TP(N)	A 240
	RHU(N)=PRHU(N)	A 241
	P(N)=PP(N)	A 242
	ETA(N)=ETAP(N)	A 243
14	TS(N)=TSP(N)	A 244
	HBRKN2=PHBRKN2	A 245
	HBRKQ2=PHBRKQ2	A 246

	L=LPP	A 247
	LP=LPPP	A 248
	DT=.75*DT	A 249
	GO TO 109	A 250
15	CONTINUE	A 251
C		A 252
C	COMPUTE MASS RATE OF PYROLYSIS GAS GENERATED AT INTERFACE	A 253
C		A 254
C	CALCULATE PYROLYSIS RATE	A 255
C	CHECK IOPTI- IOPTI=1 AND TS(I)=TIBAR USE EQ 3-42 FOR MGDOT	A 256
C	IOPTI=0 USE EQ 3-44 FOR MGDOT	A 257
	IF (NIT.GT.1) GO TO 20	A 258
	SP=1.	A 259
	IF (TS(I).LE.(TIBAR-6.)) GO TO 16	A 260
	SP=(TIBAR-TS(I))/6.	A 261
	IF (SP.LT.0.) SP=0.	A 262
16	CONTINUE	A 263
	IF ((MGDOT.GT.1.E-5).AND.(NITA.EQ.1)) GO TO 17	A 264
	NITP=0	A 265
	IF (MGDOT.GT.1.E-3) NITP=1	A 266
	IF ((NITP.EQ.1).AND.(NITA.EQ.0)) DT=.0625	A 267
17	TIME=TIME+DT	A 268
	GO TO 19	A 269
18	MGDOT=AEXP*EXP(-BEXP/TS(I))	A 270
19	CONTINUE	A 271
	IF (MGDOT.GT.0.) GO TO 21	A 272
	MGDOT=0.	A 273
	IF (IOPTI.EQ.0) GO TO 21	A 274
	TS(I)=TS(I)-1.E-4	A 275
20	CONTINUE	A 276
	IF (IOPTI.EQ.0) GO TO 18	A 277
	AMGDOT=AEXP*EXP(-BEXP/TS(I))	A 278
	BMGDOT=(-KS(I)*(11.*TS(I)-18.*TS(I+1)+9.*TS(I+2)-2.*TS(I+3)))/(6.*DX	A 279
	1*L)-KP(I)*(11.*TS(I)-18.*TS(I+1)+9.*TS(I+2)-2.*TS(I+3)))/(6.*DXP1*L	A 280
	2P))/DHP	A 281

	MGDOT=SP*AMGDOT+(1.-SP)*BMGDOT	A 282
21	CONTINUE	A 283
	MGDOT=.875*MGDOTP+.125*MGDOT	A 284
	IF (NIT.EQ.1) GO TO 22	A 285
	GO TO 26	A 286
22	CONTINUE	A 287
	IF (NITC.EQ.0) GO TO 23	A 288
	AMDOT(1)=AMDOT(1)*MGDOT/MGDOTP	A 289
23	CONTINUE	A 290
C	DETERMINE SURFACE HEATING AND PRESSURE	A 291
	CALL FTLUP (TIME,QC,MQC,NQC,TIMET,QCTAB)	A 292
	IF (IOPTP.EQ.1) GO TO 24	A 293
	PWP=5.69306E6*RAJ*(QC/HE)**2	A 294
	GO TO 25	A 295
24	CONTINUE	A 296
	CALL FTLUP (TIME,PW,MSQPT,NSQPT,TMPRES,SQPT)	A 297
	PW=PW**2	A 298
	PWP=1.013E5*PW	A 299
25	CONTINUE	A 300
	P(1)=PWP	A 301
26	CONTINUE	A 302
	AMDOT(1)=MGDOT	A 303
	DO 27 N=1,NNO	A 304
27	HKT(N)=HKT(N,8)	A 305
	CALL FTLUP (TS(1),HBRKN2,MNO,NNO,TEMP,HKT(N))	A 306
	DO 28 N=1,NNO	A 307
28	HKT(N)=HKT(N,13)	A 308
	CALL FTLUP (TS(1),HBRK02,MNO,NNO,TEMP,HKT(N))	A 309
	HW=.790795*HBRKN2+.209205*HBRK02	A 310
C	CALCULATE SURFACE REMOVAL RATE	A 311
C	CHECK IOPT1- IOPT1=1 AND TS(1)=T1BAR USE EQ 3-41 FOR MSDOT	A 312
C	IOPT1=0 USE EQ 3-36 FOR MSDOT	A 313
	IF (NIT.GT.1) GO TO 29	A 314
	S=1.	A 315
	IF (TS(1).LE.(T1BAR-22.)) GO TO 29	A 316



	S=(T1BAR-TS(1))/22.	A 317
	IF (S.LT.0.) S=0.	A 318
29	CONTINUE	A 319
	QCOND=KS(1)*(11.*TS(1)-18.*TS(2)+9.*TS(3)-2.*TS(4))/(6.*DX1*L)	A 320
	KA=AC*EXP(-BC/TS(1))	A 321
	AMSDOT=KA*PW*CE*.901/(1.+KA*PW*(HE-HW)/(.032*LAM*QCT))	A 322
	BMSDOT=(QCT+ALPHA*QRS-SGMA*EPSS*TS(1)**4-QCOND)/HC	A 323
	MSDOT=S*AMSDOT+(1.-S)*BMSDOT	A 324
	IF (MSDOT.GT.0.) GO TO 30	A 325
	MSDOT=0.	A 326
	IF (IOPT.EQ.0) GO TO 30	A 327
	TS(1)=TS(1)-1.E-4	A 328
30	CONTINUE	A 329
	MSDOT=.875*MSDOTP+.125*MSDOT	A 330
	MPDOT=ALFC*MSDOT+ALFP*AMDOT(1)	A 331
C	CALCULATE NET AERODYNAMIC HEATING RATE TO SURFACE- EQ. 3-40	A 332
	QFAC=HE*MPDOT/(QC*.029)	A 333
	IF (QFAC.GT.2.25) GO TO 31	A 334
	QCT=QC*(1.-HW/HE)*(1.-TREF*TRAB*MPDOT*HE/(QC*.029)-(1.-TRAB)*(1.724	A 335
	1*HE/(QC*.029)*MPDOT-.13*(HE*MPDOT/(QC*.029)**2))	A 336
	GO TO 32	A 337
31	QCT=QC*(1.-HW/HE)*.04	A 338
32	CONTINUE	A 339
	Q=QCT+ALPHA*QRS+S*MSDOT*DHC-(1.-S)*MSDOT*HC	A 340
	DDX=DX1	A 341
C	DETERMINE PROPERTY DATA FOR CHAR LAYER AND PYROLYSIS GASES	A 342
	IF (T(20).GT.1000.) ICHCOM=1	A 343
	X=-DDX	A 344
	IF (NIT.GT.1) GO TO 37	A 345
	DO 34 N=5,1,5	A 346
	J=N	A 347
	IF (N.EQ.5) J=1	A 348
	NSTEP=J	A 349
	IF (T(J).LT.299.) GO TO 33	A 350
C	CALL SUBROUTINE VISC TO COMPUTE VISCOSITY AND PRANDTL NUMBER OF	A 351

C	PYROLYSIS GASES	A 352
	CALL VISC	A 353
33	CONTINUE	A 354
34	CONTINUE	A 355
	DO 35 N=2,9	A 356
	ANJ=(N-1)/9.	A 357
	MU(N)=MU(1)+ANJ*(MU(10)-MU(1))	A 358
35	PR(N)=PR(1)+ANJ*(PR(10)-PR(1))	A 359
	DO 36 N=15,1,5	A 360
	KON=4	A 361
	APR=(PR(N)-PR(N-5))/5.	A 362
	AMU=(MU(N)-MU(N-5))/5.	A 363
	DO 36 J=1,4	A 364
	PR(N-KON)=PR(N-5)+J*APR	A 365
	MU(N-KON)=MU(N-5)+J*AMU	A 366
36	KON=KON-1	A 367
	PMU=MU(1)	A 368
37	CONTINUE	A 369
	DO 53 N=1,1	A 370
	CALL FTLJP (T(N),HK(N,13),MNO,NNO,TEMP,HKTV)	A 371
	AVGMF(N)=0.	A 372
	DO 38 K=1,KT	A 373
	AVGMF(N)=AVGMF(N)+MFK(N,K)*M(K)	A 374
38	CONTINUE	A 375
	IF (N.EQ.21) DDX=DX	A 376
	X=X+DDX	A 377
	VC(N)=(MSDOT/RHOSO+X*(MGDOT/DRHO-MSDOT/RHOSO))/L	A 378
	IF (NITC.EQ.0) GO TO 39	A 379
	IF (ABS(TS(N)-PTS(N)).LT.5.) GO TO 40	A 380
	PTS(N)=TS(N)	A 381
39	CONTINUE	A 382
	CALL FTLJP (TS(N),HS(N),MNO,NNO,TEMP,HSTT)	A 383
	IF (NITC.GT.0) GO TO 40	A 384
	AVGMFP(N)=AVGMF(N)	A 385
	PM(N)=PMV	A 386

	CPS(N)=CPSV	A 387
40	CONTINUE	A 388
	CALL FTLUP (TS(N),KS(N),MKS,NKS,TKS,KST)	A 389
C	NEGLECT HEAT CONDUCTION IN FLUID	A 390
	NSTEP=N	A 391
	IF (ICHCOM.EQ.0) GO TO 41	A 392
C	CALL SUBROUTINE CHCOM TO DETERMINE CHEMICAL REACTION RATES OF	A 393
C	EACH SPECIES	A 394
	CALL CHCOM (TIME)	A 395
41	CONTINUE	A 396
	IF (NITC.EQ.0) GO TO 42	A 397
	IF (ABS(T(N)-PT(N)).LT.5.) GO TO 50	A 398
	PT(N)=T(N)	A 399
	IF (T(N).LT.300.) GO TO 43	A 400
42	CONTINUE	A 401
43	CONTINUE	A 402
	CALL FTLUP (T(N),HST(N),MNO,NNO,TEMP,HSTT)	A 403
	DO 45 K=1,KM	A 404
	DO 44 J=1,NNO	A 405
	CPKTV(J)=CPKT(J,K)	A 406
	HKTV(J)=HKT(J,K)	A 407
44	CONTINUE	A 408
	CALL FTLUP (T(N),HK(N,K),MNO,NNO,TEMP,HKTV)	A 409
	CALL FTLUP (T(N),CPK(N,K),MNO,NNO,TEMP,CPKTV)	A 410
	CALL FTLUP (TS(N),DHK(N,K),MNO,NNO,TEMP,HKTV)	A 411
45	CONTINUE	A 412
	NITS=0	A 413
46	CONTINUE	A 414
	IF (T(N).GT.1500.) GO TO 47	A 415
	CPK(N,11)=(2.882035E00+2.*5.16099E-03*T(N)+3.*3.971480E-06*T(N)**2	A 416
	1-4.*3.708198E-09*T(N)**3+5.*8.949908E-13*T(N)**4)*RU	A 417
	CPK(N,12)=(3.511186E-01+2.*1.876996E-02*T(N)-3.*2.649069E-06*T(N)*	A 418
	1*2-4.*1.877262E-09*T(N)**3+5.*6.077093E-13*T(N)**4)*RU	A 419
	HK(N,11)=(2.882035E00*T(N)+5.160995E-03*T(N)**2+3.971480E-06*T(N)*	A 420
	1*3-3.708198E-09*T(N)**4+8.949908E-13*T(N)**5)*RU-1.157984E04	A 421

	HK(N,12)=(3.511186E-01*T(N)+1.876996E-02*T(N)**2-2.649069E-05*T(N)	A 422
	1**3-1.877262E-09*T(N)**4+6.077093E-13*T(N)**5)*RU+1.143849E04	A 423
	GO TO 48	A 424
47	CPK(N,11)=(1.430804E00+2.*9.444913E-03*T(N)-3.*2.348033E-06*T(N)**	A 425
	12-4.*2.968006E-10*T(N)**3-5.*1.489961E-14*T(N)**4)*RJ	A 426
	CPK(N,12)=(4.619871E00+2.*1.440481E-02*T(N)-3.*3.748451E-06*T(N)**	A 427
	12+4.*4.894085E-10*T(N)**3-5.*2.515503E-14*T(N)**4)*RU	A 428
	HK(N,11)=(1.430804E00*T(N)+9.444913E-03*T(N)**2-2.348033E-06*T(N)*	A 429
	1*3-2.968006E-10*T(N)**4-1.489961E-14*T(N)**5)*RU-1.157984E04	A 430
	HK(N,12)=(4.619871E00*T(N)+1.440481E-02*T(N)**2-3.748451E-06*T(N)*	A 431
	1*3+4.894085E-10*T(N)**4-2.515503E-14*T(N)**5)*RU+1.143849E04	A 432
48	CONTINUE	A 433
	IF (NITS.EQ.1) GO TO 49	A 434
	TSAVE=T(N)	A 435
	CPSA11=CPK(N,11)	A 436
	CPSA12=CPK(N,12)	A 437
	HSA11=HK(N,11)	A 438
	HSA12=HK(N,12)	A 439
	T(N)=TS(N)	A 440
	NITS=NITS+1	A 441
	GO TO 46	A 442
49	T(N)=TSAVE	A 443
	DHK(N,11)=HK(N,11)	A 444
	DHK(N,12)=HK(N,12)	A 445
	HK(N,11)=HSA11	A 446
	HK(N,12)=HSA12	A 447
	CPK(N,11)=CPSA11	A 448
	CPK(N,12)=CPSA12	A 449
	DHJ(N,6)=2.*DHK(N,5)-HK(N,9)-HS(N)	A 450
	DHJ(N,7)=DHK(N,5)+DHK(N,2)-HK(N,6)-HS(N)	A 451
	DHJ(N,9)=DHK(N,10)+DHK(N,2)-HK(N,7)-HS(N)	A 452
50	CONTINUE	A 453
	HRJSUM(N)=0.	A 454
	HRSUM(N)=0.	A 455
	RM(N)=0.	A 456

	ROCPM(N)=0.	A 457
	ROHM(N)=0.	A 458
	DO 51 K=1,KT	A 459
51	RM(N)=RM(N)+R(N,K)*M(K)	A 460
	DO 52 K=1,KT	A 461
	HRJSUM(N)=HRJSUM(N)+RHR(N,K)*DHJ(N,K)	A 462
	HRSUM(N)=HRSUM(N)+R(N,K)*HK(N,K)	A 463
	ROHM(N)=ROHM(N)+RHOK(N,K)*HK(N,K)/M(K)	A 464
52	ROCPM(N)=ROCPM(N)+RHOK(N,K)*CPK(N,K)/M(K)	A 465
53	CONTINUE	A 466
	DMBRDX(1)=(-11.*AVGMF(1)+18.*AVGMF(2)-9.*AVGMF(3)+2.*AVGMF(4))/(6.*DX1)	A 467
	DTDX(1)=(-11.*T(1)+18.*T(2)-9.*T(3)+2.*T(3))/(6.*DX1)	A 468
	DDX=DX1	A 469
	DO 55 N=2,IM	A 470
	IF (N.EQ.20) GO TO 54	A 471
	DMBRDX(N)=(AVGMF(N+1)-AVGMF(N-1))/(2.*DDX)	A 472
	DTDX(N)=(T(N+1)-T(N-1))/(2.*DDX)	A 473
	GO TO 55	A 474
54	DMBRDX(N)=(DX1**2*AVGMF(N+1)-(DX1**2-DX**2)*AVGMF(N)-DX**2*AVGMF(N-1))/(DX1*DX*(DX1+DX))	A 475
	DTDX(N)=(DX1**2*T(N+1)-(DX1**2-DX**2)*T(N)-DX**2*T(N-1))/(DX1*DX*(DX1+DX))	A 476
	DDX=DX	A 477
55	CONTINUE	A 478
	DMBRDX(I)=(11.*AVGMF(I)-18.*AVGMF(IM)+9.*AVGMF(I-2)-2.*AVGMF(I-3))/1/(6.*DX)	A 479
	DTDX(I)=(11.*T(I)-18.*T(IM)+9.*T(I-2)-2.*T(I-3))/(6.*DX)	A 480
	PPM=PM(I)	A 481
C	DETERMINE PROPERTIES OF UNCHARRED LAYER AND INSULATION LAYER	A 482
	DO 57 N=1,IP	A 483
	IF (NITC.EQ.0) GO TO 56	A 484
	IF (ABS(TS(N)-PTS(N)).LT.5.) GO TO 57	A 485
	PTS(N)=TS(N)	A 486
56	CONTINUE	A 487
		A 488
		A 489
		A 490
		A 491

	CALL FTLUP (TS(N),KP(N),MKP,NKP,TKP,<PT)	A 492
	CALL FTLUP (TS(N),CPP(N),MCP,NCPP,TCPP,CPPT)	A 493
	RHOP(N)=576.	A 494
57	CONTINUE	A 495
	IF (NITC.GT.0) GO TO 60	A 496
	DO 58 N=1,I	A 497
	HA(N)=PROPC*ROCPM(N)*V(N)/PR(N)	A 498
58	CONTINUE	A 499
	DO 59 N=IP,IZ	A 500
	KPP(N)=KPPV	A 501
	CPPP(N)=CPPPV	A 502
	RHOPP(N)=RHOPPV	A 503
59	CONTINUE	A 504
	KPPPIP=KPP(IP)	A 505
	KPPPIZ=KPP(IZ)	A 506
	KSP1=KS(1)	A 507
	KSPI=KS(I)	A 508
	KPPI=KP(I)	A 509
	KPPIP=KP(IP)	A 510
60	CONTINUE	A 511
	DKSDX(1)=(-11.*KS(1)+18.*KS(2)-9.*KS(3)+2.*KS(4))/(6.*DX1)	A 512
	DKSDX(I)=(11.*KS(I)-18.*KS(IM)+9.*KS(I-2)-2.*KS(I-3))/(6.*DX)	A 513
	DDX=DX1	A 514
	DO 62 N=2,IM	A 515
	IF (N.EQ.20) GO TO 61	A 516
	DKSDX(N)=(KS(N+1)-KS(N-1))/(2.*DDX)	A 517
	GO TO 62	A 518
61	DDX=DX	A 519
	DKSDX(20)=(DX1**2*KS(21)+(DX**2-DX1**2)*KS(20)-DX**2*KS(19))/(DX1*	A 520
	1DX*(DX1+DX))	A 521
62	CONTINUE	A 522
	DKPDX(I)=(-11.*KP(I)+18.*KP(IN)-9.*KP(IN2)+2.*KP(I+4))/(6.*DXP1)	A 523
	DKPDX(IP)=(11.*KP(IP)-18.*KP(IJ1)+9.*KP(IO)-2.*KP(IP-3))/(6.*DXP)	A 524
	DDX=DXP1	A 525
	DO 64 N=IN,I01	A 526

	IF (N.EQ.(I+20)) GO TO 63	A 527
	DKPDX(N)=(KP(N+1)-KP(N-1))/(2.*DXP)	A 528
	GO TO 64	A 529
63	DKPDX(I+20)=(DXP1**2*KP(I+21)+(DXP**2-DXP1**2)*KP(I+20)-DXP**2*KP(I+19)))/(DXP1*DXP*(DXP1+DXP))	A 530
	DDX=DXP	A 531
64	CONTINUE	A 532
C		A 533
C	SOLUTION OF PARTIAL DIFFERENTIAL EQUATION FOR CHAR LAYER	A 534
C		A 535
C	CALCULATE COEFFICIENTS IN DIFFERENTIAL EQ FOR SOLID TEMPERATURE	A 536
	DO 66 N=1,I	A 537
	ATS(N)=TS(N)	A 538
	ALPHA1(N)=(DKSDX(N)+L**2*(1.-ETA(N))*CPS(N)*RHOST/MS*VC(N))/KS(N)	A 539
	ALPHA2(N)=0.	A 540
	ALPHA3(N)=L**2/KS(N)*(HA(N)*(TP(N)-TSP(N))+ETA(N)*(HST(N)*RS(N)+RH	A 541
	1S(N)*HS(N)-HRJSUM(N))+RHOST*HS(N)/MS*((ETA(N)-ETAP(N))/DT-VC(N)*DE	A 542
	2TADX(N))	A 543
	ALPHA4(N)=-((1.-ETA(N))*L**2*RHOST*CPS(N)/(MS*KS(N)))	A 544
	IF (NITC.NE.0) GO TO 65	A 545
	ALPHP1(N)=ALPHA1(N)	A 546
	ALPHP2(N)=ALPHA2(N)	A 547
	ALPHP3(N)=ALPHA3(N)	A 548
	ALPHP4(N)=ALPHA4(N)	A 549
65	CONTINUE	A 550
	ALPHB3(N)=CRNI*ALPHA3(N)+(1.-CRNI)*ALPHP3(N)	A 551
	ALPHB4(N)=CRNI*ALPHA4(N)+(1.-CRNI)*ALPHP4(N)	A 552
66	CONTINUE	A 553
	IF (NITC.NE.0) GO TO 67	A 554
	ALPHI1=ALPHA1(I)	A 555
	ALPHI2=ALPHA2(I)	A 556
	ALPHI3=ALPHA3(I)	A 557
	ALPHI4=ALPHA4(I)	A 558
67	CONTINUE	A 559
	ALPHI1=ALPHA1(I)	A 560
		A 561

	ALPHI2=ALPHA2(I)	A 562
	ALPHI3=ALPHA3(I)	A 563
	ALPHI4=ALPHA4(I)	A 564
	DDX=DXP1	A 565
	XP=0.	A 566
	DO 68 N=I,IP	A 567
	IF (N.EQ.(I+20)) DDX=DXP	A 568
	ATS(N)=TS(N)	A 569
	ALPHA1(N)=(DKPDX(N)+LP*RHOP(N)*CPP(N)*MGDOT*(1.-XP)/DRHO)/KP(N)	A 570
	XP=XP+DDX	A 571
	ALPHA2(N)=0.	A 572
	ALPHA3(N)=0.	A 573
	ALPHA4(N)=-RHOP(N)*CPP(N)*LP**2/KP(N)	A 574
	ALPHB3(N)=0.	A 575
	IF (NITC.NE.0) GO TO 68	A 576
	ALPHP1(N)=ALPHA1(N)	A 577
	ALPHP2(N)=ALPHA2(N)	A 578
	ALPHP3(N)=ALPHA3(N)	A 579
	ALPHP4(N)=ALPHA4(N)	A 580
63	ALPHB4(N)=CRNI*ALPHA4(N)+(1.-CRNI)*ALPHP4(N)	A 581
	IF (NITC.NE.0) GO TO 69	A 582
	GAMMIP1=ALPHA1(I)	A 583
	GAMMIP2=ALPHA2(I)	A 584
	GAMMIP3=ALPHA3(I)	A 585
	GAMMIP4=ALPHA4(I)	A 586
	GAMIPP1=ALPHA1(IP)	A 587
	GAMIPP2=ALPHA2(IP)	A 588
	GAMIPP3=ALPHA3(IP)	A 589
	GAMIPP4=ALPHA4(IP)	A 590
69	CONTINUE	A 591
	GAMMI1=ALPHA1(I)	A 592
	GAMMI2=ALPHA2(I)	A 593
	GAMMI3=ALPHA3(I)	A 594
	GAMMI4=ALPHA4(I)	A 595



	GAMIP1=ALPHA1(IP)	A 596
	GAMIP2=ALPHA2(IP)	A 597
	GAMIP3=ALPHA3(IP)	A 598
	GAMIP4=ALPHA4(IP)	A 599
	DO 71 N=IP,IZ	A 600
	ATS(N)=TS(N)	A 601
	ALPHA1(N)=0.	A 602
	ALPHA2(N)=0.	A 603
	ALPHA3(N)=0.	A 604
	ALPHA4(N)=-RHOPP(N)*CPPP(N)*IL**2/KPP(N)	A 605
	IF (NITC.NE.0) GO TO 70	A 606
	ALPHP1(N)=ALPHA1(N)	A 607
	ALPHP2(N)=ALPHA2(N)	A 608
	ALPHP3(N)=ALPHA3(N)	A 609
	ALPHP4(N)=ALPHA4(N)	A 610
	ALPHB3(N)=0.	A 611
70	CONTINUE	A 612
71	ALPHB4(N)=CRNI*ALPHA4(N)+(1.-CRNI)*ALPHP4(N)	A 613
	IF (NITC.NE.0) GO TO 72	A 614
	KAPIPP1=ALPHA1(IP)	A 615
	KAPIPP2=ALPHA2(IP)	A 616
	KAPIPP3=ALPHA3(IP)	A 617
	KAPIPP4=ALPHA4(IP)	A 618
72	CONTINUE	A 619
	KAPIP1=ALPHA1(IP)	A 620
	KAPIP2=ALPHA2(IP)	A 621
	KAPIP3=ALPHA3(IP)	A 622
	KAPIP4=ALPHA4(IP)	A 623
C	CALL SUBROUTINE PDE1 TO SOLVE FOR TS	A 624
	CALL PDE1 (TS,CRNI)	A 625
C	CALCULATE COEFFICIENTS IN DIFFERENTIAL EQ FOR P	A 626
	DDX=DX1	A 627
	DO 74 N=1,I	A 628
	AP(N)=P(N)	A 629
	IF (N.EQ.1) GO TO 74	A 630
	PAL2(N)=2.*MU(N)*ETA(N)*L**2/(PM(N)*RHO(N)*RU*T(N))*(AVGMF(N)*(T(N	A 631

	1)-(TP(N))/(DT*T(N))-AVGMF(N)*VC(N)*DTDX(N)/T(N)+VC(N)*DMBRDX(N)-(AV	A 632
	2GMF(N)-AVGMF(N))/DT)	A 633
	PAL3(N)=2.*MU(N)*ETA(N)*P(N)*RM(N)*L**2/(PM(N)*RHO(N))	A 634
	PAL4(N)=-MU(N)*ETA(N)*AVGMF(N)*L**2/(PM(N)*RHO(N)*RU*T(N))	A 635
	IF (N.EQ.1) GO TO 74	A 636
	IF (N.EQ.20) GO TO 73	A 637
	PAL1(N)=MU(N)*ETA(N)*T(N)/(PM(N)*AVGMF(N))*(PM(N+1)*AVGMF(N+1)/(MU	A 638
	1(N+1)*ETA(N+1)*T(N+1))-PM(N-1)*AVGMF(N-1)/(MU(N-1)*ETA(N-1)*T(N-1)	A 639
	2))/(2.*DDX)+MU(N)*ETA(N)*AVGMF(N)*L**2/(PM(N)*RHO(N)*RU*T(N))*VC(N	A 640
	3)	A 641
	GO TO 74	A 642
73	CONTINUE	A 643
	DDX=DX	A 644
	PAL1(20)=MU(20)*ETA(20)*T(20)/(PM(20)*AVGMF(20))*(DX1**2*PM(21)*AV	A 645
	1GMF(21)/(MU(21)*ETA(21)*T(21))-(DX1**2-DX**2)*PM(20)*AVGMF(20)/(MU	A 646
	2(20)*ETA(20)*T(20))-DX**2*PM(19)*AVGMF(19)/(MU(19)*ETA(19)*T(19))	A 647
	3)/(DX1*DX*(DX1+DX))+MU(20)*ETA(20)*AVGMF(20)*L**2/(PM(20)*RHO(20)*T	A 648
	4(20)*RU)*VC(20)	A 649
74	CONTINUE	A 650
	PAL1(I)=MU(I)*ETA(I)*T(I)/(PM(I)*AVGMF(I))*(11.*PM(I)*AVGMF(I)/(MU	A 651
	1(I)*ETA(I)*T(I))-18.*PM(IM)*AVGMF(IM)/(MU(IM)*ETA(IM)*T(IM))+9.*PM	A 652
	2(I-2)*AVGMF(I-2)/(MU(I-2)*ETA(I-2)*T(I-2))-2.*PM(I-3)*AVGMF(I-3)/(	A 653
	3MU(I-3)*ETA(I-3)*T(I-3)))/(6.*DX)+MU(I)*ETA(I)*AVGMF(I)*L**2*VC(I)	A 654
	4/(PM(I)*RHO(I)*RU*T(I))	A 655
	DO 76 N=2,I	A 656
	IF (NITC.GT.0) GO TO 75	A 657
	PAP1(N)=0.	A 658
	PAP2(N)=0.	A 659
	PAP3(N)=0.	A 660
	PAP4(N)=0.	A 661
75	PAB3(N)=CRNI*PAL3(N)+(1.-CRNI)*PAP3(N)	A 662
76	PAB4(N)=CRNI*PAL4(N)+(1.-CRNI)*PAP4(N)	A 663
C	CALL SUBROUTINE PCP TO SOLVE FOR P	A 664
	CALL PDP (CRNI,DT,L,DX,DX1,MGDOT,MGDOTP,LPP,I,IM,RHO,P,MU,T,TP,RU)	A 665
C	CALCULATE LOCAL PYROLYSIS GAS DENSITY	A 666

	DO 77 N=1,I	A 667
	RHO(N)=P(N)*AVGMF(N)/(RU*T(N))	A 668
77	CONTINUE	A 669
	DRDDX(1)=(-11.*RHO(1)+18.*RHO(2)-9.*RHO(3)+2.*RHO(4))/(6.*DX1)	A 670
	DDX=DX1	A 671
	DO 79 N=2,IM	A 672
	IF (N.EQ.20) GO TO 78	A 673
	DRDDX(N)=(RHO(N+1)-RHO(N-1))/(2.*DDX)	A 674
	GO TO 79	A 675
78	DDX=DX	A 676
	DRDDX(N)=(DX1**2*RHO(N+1)+(DX**2-DX1**2)*RHO(N)-DX**2*RHO(N-1))/(D	A 677
	1X1*DX*(DX1+DX))	A 678
79	CONTINUE	A 679
	DRDDX(I)=(11.*RHO(I)-18.*RHO(IM)+9.*RHO(I-2)-2.*RHO(I-3))/(6.*DX)	A 680
C	CHECK PYROLYSIS RATE- IF LESS THAN MIN NEGLECT THERMAL NON-	A 681
C	EQUILIBRIUM OF PYROLYSIS GASES AND CHAR LAYER AND CHEMICAL	A 682
C	REACTIONS	A 683
	IF (NITP.GT.0) GO TO 81	A 684
	DO 80 N=1,I	A 685
	ETA(N)=ETA(I)	A 686
	AT(N)=T(N)	A 687
	T(N)=TS(N)	A 688
	AMDDOT(N)=MGDDOT	A 689
	V(N)=-MGDDOT/(RHO(N)*ETA(N))	A 690
	DO 80 K=1,KT	A 691
	RHOK(N,K)=MFK(N,K)*RHO(N)*M(K)/AVGMF(N)	A 692
80	CONTINUE	A 693
	GO TO 101	A 694
81	CONTINUE	A 695
C	CALCULATE LOCAL MASS FLOW RATE OF PYROLYSIS GASES	A 696
	AIN1(IM)=DX/2.*(ETA(I)*RHO(I)+ETA(IM)*RHO(IM))	A 697
	AIN3(IM)=DX/2.*(ETA(I)*((RHO(I)-PRHO(I))/DT-RM(I))+RHO(I)*(ETA(I)	A 698
	1-ETAP(I))/DT+ETA(IM)*((RHO(IM)-PRHO(IM))/DT-RM(IM))+RHO(IM)*(ETA(I	A 699
	2M)-ETAP(IM))/DT)	A 700
	KUN=I-2	A 701

	DDX=DX	A 702
	DO 83 N=3,I	A 703
	IF (KON.EQ.19) GO TO 82	A 704
	AINT1(KON)=AINT1(KON+2)+DDX/3.*(ETA(KON+2)*RHO(KON+2)+4.*ETA(KON+1	A 705
	1)*RHO(KON+1)+ETA(KON)*RHO(KON))	A 706
	AINT3(KON)=AINT3(KON+2)+DDX/3.*(ETA(KON+2)*((RHO(KON+2)-PRHO(KON+2	A 707
	1))/DT-RM(KON+2))+RHO(KON+2)*(ETA(KON+2)-ETAP(KON+2))/DT+4.*(ETA(KO	A 708
	2N+1)*((RHO(KON+1)-PRHO(KON+1))/DT-RM(KON+1))+RHO(KON+1)*(ETA(KON+1	A 709
	3)-ETAP(KON+1))/DT)+ETA(KON)*((RHO(KON)-PRHO(KON))/DT-RM(KON))+RHO(	A 710
	4KON)*(ETA(KON)-ETAP(KON))/DT)	A 711
	GO TO 83	A 712
82	DDX=DX1	A 713
	AINT1(KON)=AINT1(KON+1)+DDX/2.*(ETA(KON+1)*RHO(KON+1)+ETA(KON)*RHO	A 714
	1(KON))	A 715
	AINT3(KON)=AINT3(KON+1)+DDX/2.*(ETA(KON+1)*((RHO(KON+1)-PRHO(KON+1	A 716
	1))/DT-RM(KON))+RHO(KON+1)*(ETA(KON+1)-ETAP(KON+1))/DT+ETA(KON)*((R	A 717
	2HO(KON)-PRHO(KON))/DT-RM(KON))+RHO(KON)*(ETA(KON)-ETAP(KON))/DT)	A 718
83	KON=KON-1	A 719
	DO 84 N=1,IM	A 720
	AMDOT(N)=MGDOT+L*(VC(I)*ETA(I)*RHO(I)-VC(N)*ETA(N)*RHO(N))-L*AINT3	A 721
	1(N)-(MGDOT/DRHO-MSDOT/RHOSO)*AINT1(N)	A 722
84	KON=KON-1	A 723
	DO 85 N=1,I	A 724
	V(N)=-AMDOT(N)/(RHO(N)*ETA(N))	A 725
85	CONTINUE	A 726
	DO 86 N=1,I	A 727
86	DVDX(N)=L*((VC(N)-V(N)/L)*(DRODX(N)/RHO(N)+DETADX(N)/ETA(N))-((RHO	A 728
	1(N)-PRHO(N))/(DT*RHO(N))+((ETA(N)-ETAP(N))/(DT*ETA(N))+RM(N)/RHO(N)	A 729
	2))	A 730
	DO 91 K=1,KT	A 731
	NRHOK(K)=0.	A 732
	DO 87 N=1,I	A 733
	IF ((MFK(N,K).GT.1.E-5).OR.(R(N,K).GT.1.E-5)) NRHOK(K)=1	A 734
87	CONTINUE	A 735
	IF (NRHOK(K).EQ.0) GO TO 91	A 736

	ARH(I)=M(K)*MFKI(K)*MGDDOT/(AVGMF(I)*ETA(I))	A 737
C	CALCULATE COEFFICIENTS IN SPECIES CONTINUITY EQ	A 738
	DO 89 N=1,I	A 739
	BRH(N)=PAMGDDOT(N,K)	A 740
	DEN=ETA(N)*(VC(N)-V(N)/L)	A 741
	DEL1(N,K)=DETADX(N)/ETA(N)-(ETA(N)*VC(N)/V(N)*DVX(N)+(ETA(N)-ETAP	A 742
	1(N))/DT)/DEN	A 743
	DEL2(N,K)=V(N)*ETA(N)*((RHOK(N,K)-RHOKP(N,K))/DT-R(N,K)*M(K))/DEN	A 744
	DEL3(N)=0.	A 745
	IF (NITA.GT.0) GO TO 88	A 746
	DEP1(N,K)=DEL1(N,K)	A 747
	DEP2(N,K)=DEL2(N,K)	A 748
	DEP3(N)=DEL3(N)	A 749
88	DEB2(N,K)=CRNI*DEL2(N,K)+(1.-CRNI)*DEP2(N,K)	A 750
	DEB3(N)=CRNI*DEL3(N)+(1.-CRNI)*DEP3(N)	A 751
	AL1(N)=DEL1(N,K)	A 752
	AP1(N)=DEP1(N,K)	A 753
	AB2(N)=DEB2(N,K)	A 754
89	CONTINUE	A 755
C		A 756
C	COMPUTE GAS DENSITY THROUGH CHAR LAYER	A 757
C		A 758
C	CALL SUBROUTINE PDE2 TO SOLVE FOR THE LOCAL MASS FLOW OF	A 759
C	SPECIES	A 760
	CALL PDE2 (AL1,AB2,AB3,AP1,BRH,ARH,CRNI,DX,DX1,DT,I)	A 761
	DO 90 N=1,I	A 762
	IF (ARH(N).LT.1.E-100) ARH(N)=1.E-100	A 763
	RHOK(N,K)=.875*RHCKP(N,K)-.125*ARH(N)/V(N)	A 764
90	CONTINUE	A 765
91	CONTINUE	A 766
	DO 92 N=1,I	A 767
	ROM(N)=0.	A 768
	DO 92 K=1,KT	A 769
92	ROM(N)=ROM(N)+RHOK(N,K)/M(K)	A 770
	DO 93 N=1,IM	A 771

	DO 93 K=1,KT	A 772
93	MFK(N,K)=RHOK(N,K)/(ROM(N)*M(K))	A 773
C	CALCULATE COEFFICIENTS IN PYROLYSIS GAS TEMPERATURE DIFFERENTIAL	A 774
C	EQUATION	A 775
	DO 95 N=1,I	A 776
	AT(N)=T(N)	A 777
	DEN=ETA(N)*(V(N)/L-VC(N))*(ROCPM(N)-RHO(N)*RU/AVGMF(N))	A 778
	BETA1(N)=(HA(N)*TP(N)/T(N)-ETA(N)*RU*((ROM(N)-PRJM(N))/DT+(V(N)/L-	A 779
	1VC(N))*(DRODX(N)/AVGMF(N)-RHO(N)*DMBROX(N)/AVGMF(N)**2))-RHO(N)*RU	A 780
	2*((ETA(N)-ETAP(N))/DT-VC(N)*DETADX(N))/AVGMF(N))/DEN	A 781
	BETA2(N)=(ETA(N)*(HRSUM(N)-V(N)**2/2.*RM(N)+RS(N)*HST(N)+RHS(N)*HS	A 782
	1(N)-HRJSUM(N))-HA(N)*TSP(N))/DEN	A 783
	BETA3(N)=ETA(N)*(ROCPM(N)-RHO(N)*RU/AVGMF(N))/DEN	A 784
	IF (NITA.GT.0) GO TO 94	A 785
	BETP1(N)=BETA1(N)	A 786
	BETP2(N)=BETA2(N)	A 787
	BETP3(N)=BETA3(N)	A 788
94	CONTINUE	A 789
	BETB2(N)=CRNI*BETA2(N)+(1.-CRNI)*BETP2(N)	A 790
	BETB3(N)=CRNI*BETA3(N)+(1.-CRNI)*BETP3(N)	A 791
95	CONTINUE	A 792
	T(I)=TS(I)	A 793
C	CALL SUBROUTINE PDE2 TO SOLVE FOR T	A 794
	CALL PDE2 (BETA1,BETB2,BETB3,BETP1,T,T,CRNI,DX,DX1,DT,I)	A 795
	DO 96 N=1,I	A 796
C	CALCULATE COEFFICIENTS IN POROSITY DIFFERENTIAL EQUATION	A 798
96	T(N)=.875*TP(N)+.125*T(N)	A 797
	DO 98 N=1,I	A 799
	EPSA1(N)=-MS*(RHS(N)+RS(N))/(RHOST*VC(N))	A 800
	EPSA2(N)=0.	A 801
	EPSA3(N)=-1./VC(N)	A 802
	IF (NITA.NE.0) GO TO 97	A 803
	EPSP1(N)=EPSA1(N)	A 804
	EPSP3(N)=EPSA3(N)	A 805
97	CONTINUE	A 806

	EPSB3(N)=CRNI*EPSA3(N)+(1.-CRNI)*EPSP3(N)	A 807
98	CONTINUE	A 808
C	CALL SUBROUTINE PDE2 TO SOLVE FOR ETA	A 809
	CALL PDE2 (EPSA1,EPB2,EPB3,EPSP1,ETAP,ETA,CRNI,DX,DX1,DT,I)	A 810
	DETADX(1)=(-11.*ETA(1)+18.*ETA(2)-9.*ETA(3)+2.*ETA(4))/(6.*DX1)	A 811
	DDX=DX1	A 812
	DO 100 N=2,IM	A 813
	IF (N.EQ.20) GO TO 99	A 814
	DETADX(N)=(ETA(N+1)-ETA(N-1))/(2.*DDX)	A 815
	GO TO 100	A 816
99	DDX=DX	A 817
	DETADX(20)=(DX1**2*ETA(21)-(DX1**2-DX**2)*ETA(20)-DX**2*ETA(19))/(	A 818
	1DX1*DX*(DX1+DX))	A 819
100	CONTINUE	A 820
	DETADX(I)=(11.*ETA(I)-18.*ETA(IM)+9.*ETA(I-2)-2.*ETA(I-3))/(6.*DX)	A 821
	NITA=1	A 822
101	CONTINUE	A 823
	NITC=1	A 824
C	CALCULATE NEW THICKNESS VALUES FOR CHARRED AND UNCHARRED LAYERS	A 825
	DLP=(MGDOTP/DRHO+4.*(CRNI*MGDOT+(1.-CRNI)*MGDOTP)/DRHO+MGDOT/DRHO)	A 826
	1*DT/6.	A 827
	DL=DLP-(MSDOTP/(1.-ETAP(1))+4.*(CRNI*MSDOT/(1.-ETA(1))+(1.-CRNI)*M	A 828
	1SDOTP/(1.-ETAP(1)))+MSDOT/(1.-ETA(1))*DT/(6.*RHJST)	A 829
	LP=LPPP-DLP	A 830
	IF (LP.LT.LPMIN) GO TO 110	A 831
	L=LPP+DL	A 832
C	CHECK SOLUTIONS- IF NO CHECK ITERATE AGAIN	A 833
	DO 102 N=1,IZ	A 834
	IF (ABS((TS(N)-ATS(N))/TS(N)).GT.DIFER) GO TO 12	A 835
	IF (N.GT.1) GO TO 102	A 836
	IF (ABS((P(N)-AP(N))/P(N)).GT.DIFER) GO TO 12	A 837
	IF (ABS((T(N)-AT(N))/T(N)).GT.DIFER) GO TO 12	A 838
102	CONTINUE	A 839
	PART=2.*DIFER*TS(1)	A 840
	NITG=0	A 841

	IF (ABS(TS(1)-TSP(1)).GT.PART) NITG=1	A 842
	IF (ABS(TIME-PTIME-PRNTRFQ).LE.DT/2.) GO TO 103	A 843
	IF ((TIME-PTIME-PRNTRFQ).GT.0.) GO TO 103	A 844
	GO TO 105	A 845
103	CONTINUE	A 846
	QRAT=Q/QC	A 847
C	PRINT RESULTS	A 848
	WRITE (2,112) TIME,DT,NIT,TS(1),T(1),QRAT,MSDOT,MGDOT,AMDOT(1),L,L	A 849
	1P	A 850
	WRITE (2,118)	A 851
	WRITE (2,120) (TS(N),N=1,12)	A 852
	WRITE (2,113)	A 853
	WRITE (2,120) (ETA(N),N=1,1)	A 854
	WRITE (2,117)	A 855
	WRITE (2,120) (T(N),N=1,1)	A 856
	WRITE (2,119)	A 857
	WRITE (2,120) (P(N),N=1,1)	A 858
	WRITE (2,114)	A 859
	DO 104 K=1,KT	A 860
	WRITE (2,111) SPECIES(K)	A 861
	WRITE (2,120) (MEK(N,K),N=1,1)	A 862
104	CONTINUE	A 863
	WRITE (2,115)	A 864
	WRITE (2,120) (AVGMF(N),N=1,1)	A 865
	WRITE (2,116)	A 866
	WRITE (2,120) (AMDCT(N),N=1,1)	A 867
	PTIME=PTIME+10.	A 868
105	CONTINUE	A 869
C	IF SOLUTIONS CHECK RETAIN CURRENT VALUES OF PARAMETERS	A 870
	DO 108 N=1,12	A 871
	YTS(N)=(TS(N)-TSP(N))/DT	A 872
	IF (N.GT.1) GO TO 107	A 873
	YETA(N)=(ETA(N)-ETAP(N))/DT	A 874
	YRHO(N)=(RHO(N)-PRHO(N))/DT	A 875
	YP(N)=(P(N)-PP(N))/DT	A 876



	PAP1(N)=PAL1(N)	A 877
	PAP2(N)=PAL2(N)	A 878
	PAP3(N)=PAL3(N)	A 879
	PAP4(N)=PAL4(N)	A 880
	PROM(N)=ROM(N)	A 881
	PRHO(N)=RHO(N)	A 882
	AVGMFP(N)=AVGMF(N)	A 883
	PP(N)=P(N)	A 884
	EPSP1(N)=EPSA1(N)	A 885
	EPSP3(N)=EPSA3(N)	A 886
	BETP1(N)=BETA1(N)	A 887
	BETP2(N)=BETA2(N)	A 888
	BETP3(N)=BETA3(N)	A 889
	YT(N)=(T(N)-TP(N))/DT	A 890
	DEP3(N)=DEL3(N)	A 891
	DO 106 K=1,KT	A 892
	DEP1(N,K)=DEL1(N,K)	A 893
	DEP2(N,K)=DEL2(N,K)	A 894
	YRHOK(N,K)=(RHOK(N,K)-RHOKP(N,K))/DT	A 895
	PAMGDOT(N,K)=-RHOK(N,K)*V(N)	A 896
106	RHOKP(N,K)=RHOK(N,K)	A 897
	HA(N)=ABS(PFOPC*ROCPM(N)*V(N)/PR(N))	A 898
	TP(N)=T(N)	A 899
	ETAP(N)=ETA(N)	A 900
107	CONTINUE	A 901
	ALPHP1(N)=ALPHA1(N)	A 902
	ALPHP2(N)=ALPHA2(N)	A 903
	ALPHP3(N)=ALPHA3(N)	A 904
	ALPHP4(N)=ALPHA4(N)	A 905
108	TSP(N)=TS(N)	A 906
	MSDOTP=MSDOT	A 907
	ALPHIP1=ALPHI1	A 908
	ALPHIP2=ALPHI2	A 909
	ALPHIP3=ALPHI3	A 910
	ALPHIP4=ALPHI4	A 911

	GAMMIP1=GAMMI1	A 912
	GAMMIP2=GAMMI2	A 913
	GAMMIP3=GAMMI3	A 914
	GAMMIP4=GAMMI4	A 915
	GAMIPP1=GAMIP1	A 916
	GAMIPP2=GAMIP2	A 917
	GAMIPP3=GAMIP3	A 918
	GAMIPP4=GAMIP4	A 919
	KAPIPP1=KAPIP1	A 920
	KAPIPP2=KAPIP2	A 921
	KAPIPP3=KAPIP3	A 922
	KAPIPP4=KAPIP4	A 923
	QPNET=QNET	A 924
	PHBRKN2=HBRKN2	A 925
	PHBRK02=HBRK02	A 926
	QPT=Q	A 927
	KSP1=KS(1)	A 928
	KSPI=KS(I)	A 929
	KPPI=KP(I)	A 930
	KPPIP=KP(IP)	A 931
	LPP=L	A 932
	LPPP=LP	A 933
	MGDOTP=MGDOT	A 934
C	CHECK ITERATION COUNT- INCREASE TIME STEP IF ITERATION= 1	A 935
	IF (NIT.GT.1) GO TO 109	A 936
	IF (NTIME.LT.5) GO TO 109	A 937
	DT=1.5*DT	A 938
	IF (DT.GT.10) DT=10.	A 939
	NTIME=0	A 940
109	NIT=0	A 941
	NTIME=NTIME+1	A 942
	GO TO 9	A 943
110	CONTINUE	A 944
	WRITE (2,121) LP	A 945
	STOP	A 946

C		A 947
C		A 948
C		A 949
111	FORMAT (50X,A10)	A 950
112	FORMAT (/12X,7HTIME = ,F9.4,18X,5HDT = ,F7.4,24X,23HNUMBER OF ITER	A 951
	ATIONS = ,I2/12X,8HTS(1) = ,F9.2,17X,7HT(1) = ,F9.2,20X,7HQRAT = ,	A 952
	2F7.4/12X,8HMSDOT = ,E15.8,11X,8HMGDOT = ,E15.8,13X,11HAMDOT(1) = ,	A 953
	3E15.8/12X,16HCHAR THICKNESS = ,E16.3,2X,10HUNCHAR THICKNESS = ,E16.8	A 954
	4)	A 955
113	FORMAT (2X,10HCHAR LAYER POROSITY)	A 956
114	FORMAT (2X,29HMOLE FRACTION GASEOUS SPECIES)	A 957
115	FORMAT (2X,40HAVERAGE MOLECULAR WEIGHT PYROLYSIS GASES)	A 958
116	FORMAT (2X,39HLOCAL MASS FLOW RATE OF PYROLYSIS GASES)	A 959
117	FORMAT (/72X,17HFLUID TEMPERATURE)	A 960
118	FORMAT (/72X,17HSOLID TEMPERATURE)	A 961
119	FORMAT (2X,84PRESSURE)	A 962
120	FORMAT (2X,5E25.15)	A 963
121	FORMAT (20X,36HMINIMUM THICKNESS VIRGIN MATERIAL = ,E20.10)	A 964
	END	A 965-

	SUBROUTINE VISC	B	1
C	CALCULATION OF FLUID VISCOSITY AND PRANDTL NUMBER AT LOCAL TEMP-	B	2
C	ERATURE (REF. BROKAW- NASA TR R-81)	B	3
	DIMENSION MUK(12), KGK(12)	B	4
	COMMON /DE1DE2/ PSI(12,12), PHI(12,12), DUMMY(1032)	B	5
	COMMON ACEF(12), ACER(12), BCEF(12), BCER(12), CRNI, KUPT(40,12), KUPTV(	B	6
	140), M(13), MFK(50,12), MNO, NNO, MU(50), MUKT(40,12), MUKTV(40), PR(50), R	B	7
	2(50,12), RHO(50), RHOK(50,12), RHOKP(50,12), T(50), TEMP(40), NRCT, KT, RU	B	8
	3, NSTEP, RDCFM(50), RS(50)	B	9
	REAL MU, MUK, M, KUPT, MUKTV, MUKT, KUPTV, CG, KGK	B	10
	N=NSTEP	B	11
	DO 2 K=1,KT	B	12
	IF (MFK(N,K).LT.1.E-5) GO TO 2	B	13
	DO 1 J=1,NNO	B	14
	MUKTV(J)=MUKT(J,K)	B	15
	KUPTV(J)=KUPT(J,K)	B	16
1	CONTINUE	B	17
	CALL FTLUP (T(N), MUK(K), MNO, NNO, TEMP, MUKTV)	B	18
	CALL FTLJP (T(N), KGK(K), MNO, NNO, TEMP, KUPTV)	B	19
	IF (T(N).GE.300.) GO TO 2	B	20
	MUK(K)=MUKTV(1)	B	21
	KGK(K)=KUPTV(1)	B	22
2	CONTINUE	B	23
	DO 4 K=1,KT	B	24
	DO 4 J=1,KT	B	25
	IF (K.EQ.J) GO TO 4	B	26
	IF (MFK(N,K).LT.1.E-5) GO TO 3	B	27
	PHI(K,J)=(1.+SQRT(MUK(K)/MUK(J))*SQRT(SQRT(M(J)/M(K))))**2/(2.*SQR	B	28
	IT(2.)*SQRT(1.+M(K)/M(J)))	B	29
	PSI(K,J)=PHI(K,J)*(1.+2.41*(M(K)-M(J))*(M(K)-.142*M(J))/(M(K)+M(J)	B	30
	1)**2)	B	31
	GO TO 4	B	32
3	CONTINUE	B	33
	PHI(K,J)=0.	B	34
	PSI(K,J)=0.	B	35
4	CONTINUE	B	36

	MU(N)=0.	B	37
	IF (MFK(N,1).LT.1.E-5) GO TO 5	B	38
	A=1.+PHI(1,2)*RHOK(N,2)*M(1)/(RHOK(N,1)*M(2))+PHI(1,3)*RHOK(N,3)*M	B	39
	1(1)/(RHOK(N,1)*M(3))+PHI(1,4)*RHOK(N,4)*M(1)/(RHOK(N,1)*M(4))+PHI(	B	40
	21,5)*RHOK(N,5)*M(1)/(RHOK(N,1)*M(5))+PHI(1,6)*RHOK(N,6)*M(1)/(RHOK	B	41
	3(N,1)*M(6))	B	42
	MU(N)=MUK(1)/(PHI(1,7)*RHOK(N,7)*M(1)/(RHOK(N,1)*M(7))+PHI(1,8)*RH	B	43
	1OK(N,8)*M(1)/(RHOK(N,1)*M(8))+PHI(1,9)*RHOK(N,9)*M(1)/(RHOK(N,1)*M	B	44
	2(9))+PHI(1,10)*RHOK(N,10)*M(1)/(RHOK(N,1)*M(10))+PHI(1,11)*RHOK(N,	B	45
	311)*M(1)/(RHOK(N,1)*M(11))+PHI(1,12)*RHOK(N,12)*M(1)/(RHOK(N,1)*M(	B	46
	412))+A)	B	47
5	CONTINUE	B	48
	IF (MFK(N,2).LT.1.E-5) GO TO 6	B	49
	A=1.+PHI(2,1)*RHOK(N,1)*M(2)/(RHOK(N,2)*M(1))+PHI(2,3)*RHOK(N,3)*M	B	50
	1(2)/(RHOK(N,2)*M(3))+PHI(2,4)*RHOK(N,4)*M(2)/(RHOK(N,2)*M(4))+PHI(	B	51
	22,5)*RHOK(N,5)*M(2)/(RHOK(N,2)*M(5))+PHI(2,6)*RHOK(N,6)*M(2)/(RHOK	B	52
	3(N,2)*M(6))	B	53
	MU(N)=MUK(2)/(PHI(2,7)*RHOK(N,7)*M(2)/(RHOK(N,2)*M(7))+PHI(2,8)*RH	B	54
	1OK(N,8)*M(2)/(RHOK(N,2)*M(8))+PHI(2,9)*RHOK(N,9)*M(2)/(RHOK(N,2)*M	B	55
	2(9))+PHI(2,10)*RHOK(N,10)*M(2)/(RHOK(N,2)*M(10))+PHI(2,11)*RHOK(N,	B	56
	311)*M(2)/(RHOK(N,2)*M(11))+PHI(2,12)*RHOK(N,12)*M(2)/(RHOK(N,2)*M(	B	57
	412))+A)+MU(N)	B	58
6	CONTINUE	B	59
	IF (MFK(N,3).LT.1.E-5) GO TO 7	B	60
	A=1.+PHI(3,1)*RHOK(N,1)*M(3)/(RHOK(N,3)*M(1))+PHI(3,2)*RHOK(N,2)*M	B	61
	1(3)/(RHOK(N,3)*M(2))+PHI(3,4)*RHOK(N,4)*M(3)/(RHOK(N,3)*M(4))+PHI(	B	62
	23,5)*RHOK(N,5)*M(3)/(RHOK(N,3)*M(5))+PHI(3,6)*RHOK(N,6)*M(3)/(RHOK	B	63
	3(N,3)*M(6))	B	64
	MU(N)=MUK(3)/(PHI(3,7)*RHOK(N,7)*M(3)/(RHOK(N,3)*M(7))+PHI(3,8)*RH	B	65
	1OK(N,8)*M(3)/(RHOK(N,3)*M(8))+PHI(3,9)*RHOK(N,9)*M(3)/(RHOK(N,3)*M	B	66
	2(9))+PHI(3,10)*RHOK(N,10)*M(3)/(RHOK(N,3)*M(10))+PHI(3,11)*RHOK(N,	B	67
	311)*M(3)/(RHOK(N,3)*M(11))+PHI(3,12)*RHOK(N,12)*M(3)/(RHOK(N,3)*M(	B	68
	412))+A)+MU(N)	B	69
7	CONTINUE	B	70
	IF (MFK(N,4).LT.1.E-5) GO TO 8	B	71

	A=1.+PHI(4,1)*RHOK(N,1)*M(4)/(RHOK(N,4)*M(1))+PHI(4,2)*RHOK(N,2)*M	B	72
	1(4)/(RHOK(N,4)*M(2))+PHI(4,3)*RHOK(N,3)*M(4)/(RHOK(N,4)*M(3))+PHI(	B	73
	24,5)*RHOK(N,5)*M(4)/(RHOK(N,4)*M(5))+PHI(4,6)*RHOK(N,6)*M(4)/(RHOK	B	74
	3(N,4)*M(6))	B	75
	MU(N)=MUK(4)/(PHI(4,7)*RHOK(N,7)*M(4)/(RHOK(N,4)*M(7))+PHI(4,8)*RH	B	76
	1OK(N,8)*M(4)/(RHOK(N,4)*M(8))+PHI(4,9)*RHOK(N,9)*M(4)/(RHOK(N,4)*M	B	77
	2(9))+PHI(4,10)*RHOK(N,10)*M(4)/(RHOK(N,4)*M(10))+PHI(4,11)*RHOK(N,	B	78
	311)*M(4)/(RHOK(N,4)*M(11))+PHI(4,12)*RHOK(N,12)*M(4)/(RHOK(N,4)*M(	B	79
	412))+A)+MU(N)	B	80
8	CONTINUE	B	81
	IF (MFK(N,5).LT.1.E-5) GO TO 9	B	82
	A=1.+PHI(5,1)*RHOK(N,1)*M(5)/(RHOK(N,5)*M(1))+PHI(5,2)*RHOK(N,2)*M	B	83
	1(5)/(RHOK(N,5)*M(2))+PHI(5,3)*RHOK(N,3)*M(5)/(RHOK(N,5)*M(3))+PHI(	B	84
	25,4)*RHOK(N,4)*M(5)/(RHOK(N,5)*M(4))+PHI(5,6)*RHOK(N,6)*M(5)/(RHOK	B	85
	3(N,5)*M(6))	B	86
	MU(N)=MUK(5)/(PHI(5,7)*RHOK(N,7)*M(5)/(RHOK(N,5)*M(7))+PHI(5,8)*RH	B	87
	1OK(N,8)*M(5)/(RHOK(N,5)*M(8))+PHI(5,9)*RHOK(N,9)*M(5)/(RHOK(N,5)*M	B	88
	2(9))+PHI(5,10)*RHOK(N,10)*M(5)/(RHOK(N,5)*M(10))+PHI(5,11)*RHOK(N,	B	89
	311)*M(5)/(RHOK(N,5)*M(11))+PHI(5,12)*RHOK(N,12)*M(5)/(RHOK(N,5)*M(	B	90
	412))+A)+MU(N)	B	91
9	CONTINUE	B	92
	IF (MFK(N,6).LT.1.E-5) GO TO 10	B	93
	A=1.+PHI(6,1)*RHOK(N,1)*M(6)/(RHOK(N,6)*M(1))+PHI(6,2)*RHOK(N,2)*M	B	94
	1(6)/(RHOK(N,6)*M(2))+PHI(6,3)*RHOK(N,3)*M(6)/(RHOK(N,6)*M(3))+PHI(	B	95
	26,4)*RHOK(N,4)*M(6)/(RHOK(N,6)*M(4))+PHI(6,5)*RHOK(N,5)*M(6)/(RHOK	B	96
	3(N,6)*M(5))	B	97
	MU(N)=MUK(6)/(PHI(6,7)*RHOK(N,7)*M(6)/(RHOK(N,6)*M(7))+PHI(6,8)*RH	B	98
	1OK(N,8)*M(6)/(RHOK(N,6)*M(8))+PHI(6,9)*RHOK(N,9)*M(6)/(RHOK(N,6)*M	B	99
	2(9))+PHI(6,10)*RHOK(N,10)*M(6)/(RHOK(N,6)*M(10))+PHI(6,11)*RHOK(N,	B	100
	311)*M(6)/(RHOK(N,6)*M(11))+PHI(6,12)*RHOK(N,12)*M(6)/(RHOK(N,6)*M(	B	101
	412))+A)+MU(N)	B	102
10	CONTINUE	B	103
	IF (MFK(N,7).LT.1.E-5) GO TO 11	B	104
	A=1.+PHI(7,1)*RHOK(N,1)*M(7)/(RHOK(N,7)*M(1))+PHI(7,2)*RHOK(N,2)*M	B	105

	1(7)/(RHOK(N,7)*M(2))+PHI(7,3)*RHOK(N,3)*M(7)/(RHOK(N,7)*M(3))+PHI(	B	106
	27,4)*RHOK(N,4)*M(7)/(RHOK(N,7)*M(4))+PHI(7,5)*RHOK(N,5)*M(7)/(RHOK	B	107
	3(N,7)*M(5))+PHI(7,6)*RHOK(N,6)*M(7)/(RHOK(N,7)*M(6))	B	108
	MU(N)=MUK(7)/(PHI(7,8)*RHOK(N,8)*M(7)/(RHOK(N,7)*M(8))+PHI(7,9)*RH	B	109
	1OK(N,9)*M(7)/(RHOK(N,7)*M(9))+PHI(7,10)*RHOK(N,10)*M(7)/(RHOK(N,7)	B	110
	2*M(10))+PHI(7,11)*RHOK(N,11)*M(7)/(RHOK(N,7)*M(11))+PHI(7,12)*RHOK	B	111
	3(N,12)*M(7)/(RHOK(N,7)*M(12))+A)+MU(N)	B	112
11	CONTINUE	B	113
	IF (MFK(N,8).LT.1.E-5) GO TO 12	B	114
	A=1.+PHI(8,1)*RHOK(N,1)*M(8)/(RHOK(N,8)*M(1))+PHI(8,2)*RHOK(N,2)*M	B	115
	1(8)/(RHOK(N,8)*M(2))+PHI(8,3)*RHOK(N,3)*M(8)/(RHOK(N,8)*M(3))+PHI(	B	116
	28,4)*RHOK(N,4)*M(8)/(RHOK(N,8)*M(4))+PHI(8,5)*RHOK(N,5)*M(8)/(RHOK	B	117
	3(N,8)*M(5))+PHI(8,6)*RHOK(N,6)*M(8)/(RHOK(N,8)*M(6))	B	118
	MU(N)=MUK(8)/(PHI(8,7)*RHOK(N,7)*M(8)/(RHOK(N,8)*M(7))+PHI(8,9)*RH	B	119
	1OK(N,9)*M(8)/(RHOK(N,8)*M(9))+PHI(8,10)*RHOK(N,10)*M(8)/(RHOK(N,8)	B	120
	2*M(10))+PHI(8,11)*RHOK(N,11)*M(8)/(RHOK(N,8)*M(11))+PHI(8,12)*RHOK	B	121
	3(N,12)*M(8)/(RHOK(N,8)*M(12))+A)+MU(N)	B	122
12	CONTINUE	B	123
	IF (MFK(N,9).LT.1.E-5) GO TO 13	B	124
	A=1.+PHI(9,1)*RHOK(N,1)*M(9)/(RHOK(N,9)*M(1))+PHI(9,2)*RHOK(N,2)*M	B	125
	1(9)/(RHOK(N,9)*M(2))+PHI(9,3)*RHOK(N,3)*M(9)/(RHOK(N,9)*M(3))+PHI(	B	126
	29,4)*RHOK(N,4)*M(9)/(RHOK(N,9)*M(4))+PHI(9,5)*RHOK(N,5)*M(9)/(RHOK	B	127
	3(N,9)*M(5))+PHI(9,6)*RHOK(N,6)*M(9)/(RHOK(N,9)*M(6))	B	128
	MU(N)=MUK(9)/(PHI(9,7)*RHOK(N,7)*M(9)/(RHOK(N,9)*M(7))+PHI(9,8)*RH	B	129
	1OK(N,8)*M(9)/(RHOK(N,9)*M(8))+PHI(9,10)*RHOK(N,10)*M(9)/(RHOK(N,9)	B	130
	2*M(10))+PHI(9,11)*RHOK(N,11)*M(9)/(RHOK(N,9)*M(11))+PHI(9,12)*RHOK	B	131
	3(N,12)*M(9)/(RHOK(N,9)*M(12))+A)+MU(N)	B	132
13	CONTINUE	B	133
	IF (MFK(N,10).LT.1.E-5) GO TO 14	B	134
	A=1.+PHI(10,1)*RHOK(N,1)*M(10)/(RHOK(N,10)*M(1))+PHI(10,2)*RHOK(N,	B	135
	12)*M(10)/(RHOK(N,10)*M(2))+PHI(10,3)*RHOK(N,3)*M(10)/(RHOK(N,10)*M	B	136
	2(3))+PHI(10,4)*RHOK(N,4)*M(10)/(RHOK(N,10)*M(4))+PHI(10,5)*RHOK(N,	B	137
	35)*M(10)/(RHOK(N,10)*M(5))+PHI(10,6)*RHOK(N,6)*M(10)/(RHOK(N,10)*M	B	138
	4(6))	B	139
	MU(N)=MUK(10)/(PHI(10,7)*RHOK(N,7)*M(10)/(RHOK(N,10)*M(7))+PHI(10,	B	140
	18)*RHOK(N,8)*M(10)/(RHOK(N,10)*M(8))+PHI(10,9)*RHOK(N,9)*M(10)/(RH	B	141

	20K(N,10)*M(9))+PHI(10,11)*RHOK(N,11)*M(10)/(RHOK(N,10)*M(11))+PHI(	B 142
	310,12)*RHOK(N,12)*M(10)/(RHOK(N,10)*M(12))+A)+MU(N)	B 143
14	CONTINUE	B 144
	IF (MFK(N,11).LT.1.E-5) GO TO 15	B 145
	A=1.+PHI(11,1)*RHOK(N,1)*M(11)/(RHOK(N,11)*M(1))+PHI(11,2)*RHOK(N,	B 146
	12)*M(11)/(RHOK(N,11)*M(2))+PHI(11,3)*RHOK(N,3)*M(11)/(RHOK(N,11)*M	B 147
	2(3))+PHI(11,4)*RHOK(N,4)*M(11)/(RHOK(N,11)*M(4))+PHI(11,5)*RHOK(N,	B 148
	35)*M(11)/(RHOK(N,11)*M(5))+PHI(11,6)*RHOK(N,6)*M(11)/(RHOK(N,11)*M	B 149
	4(6))	B 150
	MU(N)=MUK(11)/(PHI(11,7)*RHOK(N,7)*M(11)/(RHOK(N,11)*M(7))+PHI(11,	B 151
	18)*RHOK(N,8)*M(11)/(RHOK(N,11)*M(8))+PHI(11,9)*RHOK(N,9)*M(11)/(RH	B 152
	20K(N,11)*M(9))+PHI(11,10)*RHOK(N,10)*M(11)/(RHOK(N,11)*M(10))+PHI(	B 153
	311,12)*RHOK(N,12)*M(11)/(RHOK(N,11)*M(12))+A)+MU(N)	B 154
15	CONTINUE	B 155
	IF (MFK(N,12).LT.1.E-5) GO TO 16	B 156
	A=1.+PHI(12,1)*RHOK(N,1)*M(12)/(RHOK(N,12)*M(1))+PHI(12,2)*RHOK(N,	B 157
	12)*M(12)/(RHOK(N,12)*M(2))+PHI(12,3)*RHOK(N,3)*M(12)/(RHOK(N,12)*M	B 158
	2(3))+PHI(12,4)*RHOK(N,4)*M(12)/(RHOK(N,12)*M(4))+PHI(12,5)*RHOK(N,	B 159
	35)*M(12)/(RHOK(N,12)*M(5))+PHI(12,6)*RHOK(N,6)*M(12)/(RHOK(N,12)*M	B 160
	4(6))	B 161
	MU(N)=MUK(12)/(PHI(12,7)*RHOK(N,7)*M(12)/(RHOK(N,12)*M(7))+PHI(12,	B 162
	18)*RHOK(N,8)*M(12)/(RHOK(N,12)*M(8))+PHI(12,9)*RHOK(N,9)*M(12)/(RH	B 163
	20K(N,12)*M(9))+PHI(12,10)*RHOK(N,10)*M(12)/(RHOK(N,12)*M(10))+PHI(	B 164
	312,11)*RHOK(N,11)*M(12)/(RHOK(N,12)*M(11))+A)+MU(N)	B 165
16	CONTINUE	B 166
	KG=0.	B 167
	IF (MFK(N,1).LT.1.E-5) GO TO 17	B 168
	A=(1.+PSI(1,2)*RHOK(N,2)*M(1)/(RHOK(N,1)*M(2))+PSI(1,3)*RHOK(N,3)*	B 169
	1M(1)/(RHOK(N,1)*M(3))+PSI(1,4)*RHOK(N,4)*M(1)/(RHOK(N,1)*M(4))+PSI	B 170
	2(1,5)*RHOK(N,5)*M(1)/(RHOK(N,1)*M(5))+PSI(1,6)*RHOK(N,6)*M(1)/(RHO	B 171
	3K(N,1)*M(6))	B 172
	KG=KGK(1)/(PSI(1,7)*RHOK(N,7)*M(1)/(RHOK(N,1)*M(7))+PSI(1,8)*RHOK(	B 173
	1N,8)*M(1)/(RHOK(N,1)*M(8))+PSI(1,9)*RHOK(N,9)*M(1)/(RHOK(N,1)*M(9)	B 174
	2)+PSI(1,10)*RHOK(N,10)*M(1)/(RHOK(N,1)*M(10))+PSI(1,11)*RHOK(N,11)	B 175
	3*M(1)/(RHOK(N,1)*M(11))+PSI(1,12)*RHOK(N,12)*M(1)/(RHOK(N,1)*M(12)	B 176



	4)+A)	B 177
17	CONTINUE	B 178
	IF (MFK(N,2).LT.1.E-5) GO TO 18	B 179
	A=(1.+PSI(2,1)*RHOK(N,1)*M(2)/(RHOK(N,2)*M(1))+PSI(2,3)*RHOK(N,3)*	B 180
	1M(2)/(RHOK(N,2)*M(3))+PSI(2,4)*RHOK(N,4)*M(2)/(RHOK(N,2)*M(4))+PSI	B 181
	2(2,5)*RHOK(N,5)*M(2)/(RHOK(N,2)*M(5))+PSI(2,6)*RHOK(N,6)*M(2)/(RHO	B 182
	3K(N,2)*M(6)))	B 183
	KG=KGK(2)/(PSI(2,7)*RHOK(N,7)*M(2)/(RHOK(N,2)*M(7))+PSI(2,8)*RHOK(	B 184
	1N,8)*M(2)/(RHOK(N,2)*M(8))+PSI(2,9)*RHOK(N,9)*M(2)/(RHOK(N,2)*M(9)	B 185
	2)+PSI(2,10)*RHOK(N,10)*M(2)/(RHOK(N,2)*M(10))+PSI(2,11)*RHOK(N,11)	B 186
	3*M(2)/(RHOK(N,2)*M(11))+PSI(2,12)*RHOK(N,12)*M(2)/(RHOK(N,2)*M(12)	B 187
	4)+A)+KG	B 188
18	CONTINUE	B 189
	IF (MFK(N,3).LT.1.E-5) GO TO 19	B 190
	A=(1.+PSI(3,1)*RHOK(N,1)*M(3)/(RHOK(N,3)*M(1))+PSI(3,2)*RHOK(N,2)*	B 191
	1M(3)/(RHOK(N,3)*M(2))+PSI(3,4)*RHOK(N,4)*M(3)/(RHOK(N,3)*M(4))+PSI	B 192
	2(3,5)*RHOK(N,5)*M(3)/(RHOK(N,3)*M(5))+PSI(3,6)*RHOK(N,6)*M(3)/(RHO	B 193
	3K(N,3)*M(6)))	B 194
	KG=KGK(3)/(PSI(3,7)*RHOK(N,7)*M(3)/(RHOK(N,3)*M(7))+PSI(3,8)*RHOK(	B 195
	1N,8)*M(3)/(RHOK(N,3)*M(8))+PSI(3,9)*RHOK(N,9)*M(3)/(RHOK(N,3)*M(9)	B 196
	2)+PSI(3,10)*RHOK(N,10)*M(3)/(RHOK(N,3)*M(10))+PSI(3,11)*RHOK(N,11)	B 197
	3*M(3)/(RHOK(N,3)*M(11))+PSI(3,12)*RHOK(N,12)*M(3)/(RHOK(N,3)*M(12)	B 198
	4)+A)+KG	B 199
19	CONTINUE	B 200
	IF (MFK(N,4).LT.1.E-5) GO TO 20	B 201
	A=(1.+PSI(4,1)*RHOK(N,1)*M(4)/(RHOK(N,4)*M(1))+PSI(4,2)*RHOK(N,2)*	B 202
	1M(4)/(RHOK(N,4)*M(2))+PSI(4,3)*RHOK(N,3)*M(4)/(RHOK(N,4)*M(3))+PSI	B 203
	2(4,5)*RHOK(N,5)*M(4)/(RHOK(N,4)*M(5))+PSI(4,6)*RHOK(N,6)*M(4)/(RHO	B 204
	3K(N,4)*M(6)))	B 205
	KG=KGK(4)/(PSI(4,7)*RHOK(N,7)*M(4)/(RHOK(N,4)*M(7))+PSI(4,8)*RHOK(	B 206
	1N,8)*M(4)/(RHOK(N,4)*M(8))+PSI(4,9)*RHOK(N,9)*M(4)/(RHOK(N,4)*M(9)	B 207
	2)+PSI(4,10)*RHOK(N,10)*M(4)/(RHOK(N,4)*M(10))+PSI(4,11)*RHOK(N,11)	B 208
	3*M(4)/(RHOK(N,4)*M(11))+PSI(4,12)*RHOK(N,12)*M(4)/(RHOK(N,4)*M(12)	B 209
	4)+A)+KG	B 210
20	CONTINUE	B 211

	IF (MFK(N,5).LT.1.E-5) GO TO 21	B 212
	A=(1.+PSI(5,1)*RHOK(N,1)*M(5)/(RHOK(N,5)*M(1))+PSI(5,2)*RHOK(N,2)*	B 213
	1M(5)/(RHOK(N,5)*M(2))+PSI(5,3)*RHOK(N,3)*M(5)/(RHOK(N,5)*M(3))+PSI	B 214
	2(5,4)*RHOK(N,4)*M(5)/(RHOK(N,5)*M(4))+PSI(5,6)*RHOK(N,6)*M(5)/(RHO	B 215
	3K(N,5)*M(6)))	B 216
	KG=KGK(5)/(PSI(5,7)*RHOK(N,7)*M(5)/(RHOK(N,5)*M(7))+PSI(5,8)*RHOK(	B 217
	1N,8)*M(5)/(RHOK(N,5)*M(8))+PSI(5,9)*RHOK(N,9)*M(5)/(RHOK(N,5)*M(9)	B 218
	2)+PSI(5,10)*RHOK(N,10)*M(5)/(RHOK(N,5)*M(10))+PSI(5,11)*RHOK(N,11)	B 219
	3*M(5)/(RHOK(N,5)*M(11))+PSI(5,12)*RHOK(N,12)*M(5)/(RHOK(N,5)*M(12)	B 220
	4)+A)+KG	B 221
21	CONTINUE	B 222
	IF (MFK(N,6).LT.1.E-5) GO TO 22	B 223
	A=(1.+PSI(6,1)*RHOK(N,1)*M(6)/(RHOK(N,6)*M(1))+PSI(6,2)*RHOK(N,2)*	B 224
	1M(6)/(RHOK(N,6)*M(2))+PSI(6,3)*RHOK(N,3)*M(6)/(RHOK(N,6)*M(3))+PSI	B 225
	2(6,4)*RHOK(N,4)*M(6)/(RHOK(N,6)*M(4))+PSI(6,5)*RHOK(N,5)*M(6)/(RHO	B 226
	3K(N,6)*M(5)))	B 227
	KG=KGK(6)/(PSI(6,7)*RHOK(N,7)*M(6)/(RHOK(N,6)*M(7))+PSI(6,8)*RHOK(	B 228
	1N,8)*M(6)/(RHOK(N,6)*M(8))+PSI(6,9)*RHOK(N,9)*M(6)/(RHOK(N,6)*M(9)	B 229
	2)+PSI(6,10)*RHOK(N,10)*M(6)/(RHOK(N,6)*M(10))+PSI(6,11)*RHOK(N,11)	B 230
	3*M(6)/(RHOK(N,6)*M(11))+PSI(6,12)*RHOK(N,12)*M(6)/(RHOK(N,6)*M(12)	B 231
	4)+A)+KG	B 232
22	CONTINUE	B 233
	IF (MFK(N,7).LT.1.E-5) GO TO 23	B 234
	A=(PSI(7,1)*RHOK(N,1)*M(7)/(RHOK(N,7)*M(1))+PSI(7,2)*RHOK(N,2)*M(7)	B 235
	1)/(RHOK(N,7)*M(2))+PSI(7,3)*RHOK(N,3)*M(7)/(RHOK(N,7)*M(3))+PSI(7,	B 236
	24)*RHOK(N,4)*M(7)/(RHOK(N,7)*M(4))+PSI(7,5)*RHOK(N,5)*M(7)/(RHOK(N	B 237
	3,7)*M(5))+PSI(7,6)*RHOK(N,6)*M(7)/(RHOK(N,7)*M(6)))	B 238
	KG=KGK(7)/(1.+PSI(7,8)*RHOK(N,8)*M(7)/(RHOK(N,7)*M(8))+PSI(7,9)*RH	B 239
	1OK(N,9)*M(7)/(RHOK(N,7)*M(9))+PSI(7,10)*RHOK(N,10)*M(7)/(RHOK(N,7)	B 240
	2*M(10))+PSI(7,11)*RHOK(N,11)*M(7)/(RHOK(N,7)*M(11))+PSI(7,12)*RHOK	B 241
	3(N,12)*M(7)/(RHOK(N,7)*M(12))+A)+KG	B 242
23	CONTINUE	B 243
	IF (MFK(N,8).LT.1.E-5) GO TO 24	B 244
	A=(PSI(8,1)*RHOK(N,1)*M(8)/(RHOK(N,8)*M(1))+PSI(8,2)*RHOK(N,2)*M(8	B 245
	1)/(RHOK(N,8)*M(2))+PSI(8,3)*RHOK(N,3)*M(8)/(RHOK(N,8)*M(3))+PSI(8,	B 246

	24)*RHOK(N,4)*M(8)/(RHOK(N,8)*M(4))+PSI(8,5)*RHOK(N,5)*M(8)/(RHOK(N	B 247
	3,8)*M(5))+PSI(8,6)*RHOK(N,5)*M(8)/(RHOK(N,8)*M(6)))	B 248
	KG=KGK(8)/(1+PSI(8,7)*RHOK(N,7)*M(8)/(RHOK(N,8)*M(7))+PSI(8,9)*RHO	B 249
	1K(N,9)*M(8)/(RHOK(N,8)*M(9))+PSI(8,10)*RHOK(N,10)*M(8)/(RHOK(N,8)*	B 250
	2M(10))+PSI(8,11)*RHOK(N,11)*M(8)/(RHOK(N,8)*M(11))+PSI(8,12)*RHOK(	B 251
	3N,12)*M(8)/(RHOK(N,8)*M(12))+A)+KG	B 252
24	CONTINUE	B 253
	IF (MFK(N,9).LT.1.E-5) GO TO 25	B 254
	A=(PSI(9,1)*RHOK(N,1)*M(9)/(RHOK(N,9)*M(1))+PSI(9,2)*RHOK(N,2)*M(9	B 255
	1)/(RHOK(N,9)*M(2))+PSI(9,3)*RHOK(N,3)*M(9)/(RHOK(N,9)*M(3))+PSI(9,	B 256
	24)*RHOK(N,4)*M(9)/(RHOK(N,9)*M(4))+PSI(9,5)*RHOK(N,5)*M(9)/(RHOK(N	B 257
	3,9)*M(5))+PSI(9,6)*RHOK(N,6)*M(9)/(RHOK(N,9)*M(6)))	B 258
	KG=KGK(9)/(1+PSI(9,7)*RHOK(N,7)*M(9)/(RHOK(N,9)*M(7))+PSI(9,8)*RHO	B 259
	1K(N,8)*M(9)/(RHOK(N,9)*M(8))+PSI(9,10)*RHOK(N,10)*M(9)/(RHOK(N,9)*	B 260
	2M(10))+PSI(9,11)*RHOK(N,11)*M(9)/(RHOK(N,9)*M(11))+PSI(9,12)*RHOK(	B 261
	3N,12)*M(9)/(RHOK(N,9)*M(12))+A)+KG	B 262
25	CONTINUE	B 263
	IF (MFK(N,10).LT.1.E-5) GO TO 26	B 264
	A=(PSI(10,1)*RHOK(N,1)*M(10)/(RHOK(N,10)*M(1))+PSI(10,2)*RHOK(N,2)	B 265
	1*M(10)/(RHOK(N,10)*M(2))+PSI(10,3)*RHOK(N,3)*M(10)/(RHOK(N,10)*M(3	B 266
	2))+PSI(10,4)*RHOK(N,4)*M(10)/(RHOK(N,10)*M(4))+PSI(10,5)*RHOK(N,5)	B 267
	3*M(10)/(RHOK(N,10)*M(5))+PSI(10,6)*RHOK(N,6)*M(10)/(RHOK(N,10)*M(6	B 268
	4)))	B 269
	KG=KGK(10)/(1.+PSI(10,7)*RHOK(N,7)*M(10)/(RHOK(N,10)*M(7))+PSI(10,	B 270
	18)*RHOK(N,8)*M(10)/(RHOK(N,10)*M(8))+PSI(10,9)*RHOK(N,9)*M(10)/(RH	B 271
	2OK(N,10)*M(9))+PSI(10,11)*RHOK(N,11)*M(10)/(RHOK(N,10)*M(11))+PSI(	B 272
	310,12)*RHOK(N,12)*M(10)/(RHOK(N,10)*M(12))+A)+KG	B 273
26	CONTINUE	B 274
	IF (MFK(N,11).LT.1.E-5) GO TO 27	B 275
	A=(PSI(11,1)*RHOK(N,1)*M(11)/(RHOK(N,11)*M(1))+PSI(11,2)*RHOK(N,2)	B 276
	1*M(11)/(RHOK(N,11)*M(2))+PSI(11,3)*RHOK(N,3)*M(11)/(RHOK(N,11)*M(3	B 277
	2))+PSI(11,4)*RHOK(N,4)*M(11)/(RHOK(N,11)*M(4))+PSI(11,5)*RHOK(N,5)	B 278
	3*M(11)/(RHOK(N,11)*M(5))+PSI(11,6)*RHOK(N,6)*M(11)/(RHOK(N,11)*M(6	B 279
	4)))	B 280
	KG=KGK(11)/(1.+PSI(11,7)*RHOK(N,7)*M(11)/(RHOK(N,11)*M(7))+PSI(11,	B 281

	18)*RHOK(N,8)*M(11)/(RHOK(N,11)*M(8))+PSI(11,9)*RHOK(N,9)*M(11)/(RH	B 282
	20K(N,11)*M(9))+PSI(11,10)*RHOK(N,10)*M(11)/(RHOK(N,11)*M(10))+PSI(	B 283
	311,12)*RHOK(N,12)*M(11)/(RHOK(N,11)*M(12))+A)+KG	B 284
27	CONTINUE	B 285
	IF (MFK(N,12).LT.1.E-5) GO TO 28	B 286
	A=(PSI(12,1)*RHOK(N,1)*M(12)/(RHOK(N,12)*M(1))+PSI(12,2)*RHOK(N,2)	B 287
	1*M(12)/(RHOK(N,12)*M(2))+PSI(12,3)*RHOK(N,3)*M(12)/(RHOK(N,12)*M(3	B 288
	2))+PSI(12,4)*RHOK(N,4)*M(12)/(RHOK(N,12)*M(4))+PSI(12,5)*RHOK(N,5)	B 289
	3*M(12)/(RHOK(N,12)*M(5))+PSI(12,6)*RHOK(N,6)*M(12)/(RHOK(N,12)*M(6	B 290
	4)))	B 291
	KG=KGK(12)/(1.+PSI(12,7)*RHOK(N,7)*M(12)/(RHOK(N,12)*M(7))+PSI(12,	B 292
	18)*RHOK(N,8)*M(12)/(RHOK(N,12)*M(8))+PSI(12,9)*RHOK(N,9)*M(12)/(RH	B 293
	20K(N,12)*M(9))+PSI(12,10)*RHOK(N,10)*M(12)/(RHOK(N,12)*M(10))+PSI(	B 294
	312,11)*RHOK(N,11)*M(12)/(RHOK(N,12)*M(11))+A)+KG	B 295
28	CONTINUE	B 296
	PR(N)=MU(N)/KG*ROCPM(N)/RHO(N)	B 297
	RETURN	B 298
	END	B 299-

	SUBROUTINE PDE1 (FS,CRNI)	C	1
C	SUBROUTINE FOR SOLVING SECOND ORDER LINEARIZED DIFFERENTIAL EQUA-	C	2
C	TIONS FOR TEMPERATURE OF THE CHAR AND UNCHARRED LAYERS.	C	3
	DIMENSION AS(110), BS(110), CS(110), DS(110), BP(110), FS(110), GP	C	4
	1(110), ALPHB4(110), ALPHA2(110), ALPHB3(110), TSP(110), ALPHP2(110	C	5
	2), KS(50), ALPHP1(110), ALPHA1(110), TP(50), KP(100), KPP(110), TF	C	6
	3S(110), ALPHA3(110), ALPHA4(110), ALPHP3(110), ALPHP4(110)	C	7
	COMMON /DEIDE2/ AS,BS,CS,DS,BP,GP	C	8
	COMMON /PDE1/ ALPHI1,ALPHI2,ALPHI3,ALPHI4,ALPHIP1,ALPHIP2,ALPHIP3,	C	9
	1ALPHIP4,GAMMI1,GAMMI2,GAMMI4,GAMMIP1,GAMMIP2,GAMMIP3,GAMMIP4,SGMA,	C	10
	2DX,ALPHA1,ALPHA2,ALPHP1,ALPHP2,ALPHB3,ALPHB4,DT,L,Q,KS,LP,QPT,KSP1	C	11
	3,TSP,DXP,IP,I,IO,IN,IO1,KP,LPP,LPPP,KSPI,KPPI,MGDOT,DHP,MGDOTP,QNE	C	12
	4T,QPNET,KPPIP,GAMMI3,IM,EPSS,EPSP,DX1,DXP1,ALPHA4,ALPHP3,ALPHP4,AL	C	13
	5PHA3,HTSK,HTSKP,IOPT1,IOPTI,T1BAR,TIBAR	C	14
	COMMON /TS/ IP1,IZ1,KPP,GAMIP1,GAMIP2,GAMIP3,GAMIP4,GAMIPP1,GAMIPP	C	15
	12,GAMIPP3,GAMIPP4,KAPIP1,KAPIP2,KAPIP3,KAPIP4,KAPIPP1,KAPIPP2,IL,K	C	16
	2APIPP3,KAPIPP4,DXPP,KPPPIP,KPPPIZ,IZ	C	17
	DOUBLE PRECISION AS,BS,CS,DS,GSCNST,HSCNST,AISCNST,ZSCNST,YSCNST,X	C	18
	1SCNST,AIS,BIS,CIS,DIS,BP,GP,WS,TFS	C	19
	REAL KS,KP,L,LP,MGDOT,LPP,LPPP,MGDOTP,KPPI,KSPI,XSP1,KPPIP,KAPIP1,	C	20
	1KAPIP2,KAPIP3,KAPIP4,KAPIPP1,KAPIPP2,KAPIPP3,KAPIPP4,IL,KPPPIZ,KPP	C	21
	2PIP,KPP	C	22
C	CALCULATE TRI-DIAGONAL MATRIX COEFFICIENTS	C	23
	DDX=DX1	C	24
	IF (IOPT1.EQ.0) GO TO 1	C	25
	IF ((FS(1)-T1BAR).GT.1.E-6) GO TO 2	C	26
1	CONTINUE	C	27
	BS(1)=CRNI*((ALPHA1(1)-11./(6.*DDX))*L*SGMA*EPSS*FS(1)**3/KS(1)-3.	C	28
	1/(2.*DDX**2)+ALPHA2(1))+ALPHB4(1)/DT	C	29
	CS(1)=3.*CRNI/(4.*DDX**2)	C	30
	GSCNST=CRNI*(3./(2.*DDX**2)-1./(6.*DDX**2))	C	31
	HSCNST=-3.*CRNI/(4.*DDX**2)	C	32
	AISCNST=CRNI/(6.*DDX**2)	C	33
	DS(1)=-ALPHB3(1)+CRNI*(ALPHA1(1)-11./(6.*DDX))*Q*L/KS(1)+(1.-CRNI)	C	34
	1*(ALPHP1(1)-11./(6.*DDX))*QPT*LPP/KSP1-((1.-CRNI)*((ALPHP1(1)-11./	C	35
	2(6.*DDX))*LPP*SGMA*EPSS*TSP(1)**3/KSP1-3./(2.*DDX**2)+ALPHP2(1))-A	C	36

	3ALPHB4(1)/DT)*TSP(1)-(1.-CRNI)*(3./(4.*DDX**2)*TSP(2)+(3./(2.*DDX**	C	37
	42)-1./(6.*DDX**2))*TSP(3)-3./(4.*DDX**2)*TSP(4)+1./(6.*DDX**2)*TSP	C	38
	5(5))	C	39
	GO TO 3	C	40
2	CONTINUE	C	41
	BS(1)=1.	C	42
	CS(1)=0.	C	43
	GSCNST=0.	C	44
	HSCNST=0.	C	45
	AISCNST=0.	C	46
	DS(1)=T1BAR+1.E-4	C	47
3	CONTINUE	C	48
	DO 5 N=2,IM	C	49
	IF (N.NE.20) GO TO 4	C	50
	DDX=DX	C	51
	GO TO 5	C	52
4	AS(N)=CRNI*(1./DDX**2-ALPHA1(N)/(2.*DDX))	C	53
	BS(N)=CRNI*(ALPHA2(N)-2./DDX**2+ALPHB3(N)/(DT*CRNI))	C	54
	CS(N)=CRNI*(1./DDX**2+ALPHA1(N)/(2.*DDX))	C	55
	DS(N)=-ALPHB3(N)-(1-CRNI)*((1./DDX**2-ALPHP1(N)/(2.*DDX))*TSP(N-1)	C	56
	1+(ALPHP2(N)-2./DDX**2-ALPHB4(N)/(DT*(1.-CRNI)))*TSP(N)+(1./DDX**2+	C	57
	2ALPHP1(N)/(2.*DDX))*TSP(N+1))	C	58
5	CONTINUE	C	59
	BS(1)=AS(2)/CS(2)*(CS(3)*CS(4)*GSCNST-AS(4)*CS(3)*AISCNST-BS(3)*(C	C	60
	1S(4)*HSCNST-BS(4)*AISCNST))-CS(3)*CS(4)*BS(1)	C	61
	CS(1)=BS(2)/CS(2)*(CS(3)*CS(4)*GSCNST-AS(4)*CS(3)*AISCNST-BS(3)*(C	C	62
	1S(4)*HSCNST-BS(4)*AISCNST))-CS(1)*CS(3)*CS(4)+AS(3)*(CS(4)*HSCNST-	C	63
	2BS(4)*AISCNST)	C	64
	DS(1)=DS(2)/CS(2)*(CS(3)*CS(4)*GSCNST-AS(4)*CS(3)*AISCNST-BS(3)*(C	C	65
	1S(4)*HSCNST-BS(4)*AISCNST))-CS(3)*CS(4)*DS(1)+CS(3)*DS(4)*AISCNST+	C	66
	2DS(3)*(CS(4)*HSCNST-BS(4)*AISCNST)	C	67
	AS(20)=CRNI*(ALPHA1(20)*DX/(DX1*(DX1+DX))-2./(DX1*(DX1+DX)))	C	68
	BS(20)=CRNI*(2./(DX*DX1)-ALPHA2(20)-ALPHA1(20)*(DX-DX1)/(DX1*DX))-	C	69
	1ALPHB4(20)/DT	C	70
	CS(20)=CRNI*(-2./(DX*(DX1+DX))-ALPHA1(20)*DX1/(DX*(DX1+DX)))	C	71

	DS(20)=-ALPHB3(20)-(1.-CRNI)*(ALPHP1(20)*DX/(DX1*(DX1+DX))-2./(DX1	C	72
	1*(DX1+DX))*TSP(19)-((1.-CRNI)*(2./(DX*DX1)-ALPHP2(20)-ALPHP1(20)*	C	73
	2(DX-DX1)/(DX1*DX))+ALPHB4(20)/DT)*TSP(20)+(1.-CRNI)*(2./(DX*(DX1+D	C	74
	3X))+ALPHP1(20)*DX1/(DX*(DX1+DX))*TSP(21)	C	75
	DDX=DXP1	C	76
	DO 7 N=IN,IC1	C	77
	IF (N.EQ.(I+20)) GO TO 6	C	78
	AS(N)=CRNI*(1./DDX**2-ALPHA1(N)/(2.*DDX))	C	79
	BS(N)=CRNI*(ALPHA2(N)-2./DDX**2+ALPHB4(N)/(DT*CRNI))	C	80
	CS(N)=CRNI*(1./DDX**2+ALPHA1(N)/(2.*DDX))	C	81
	DS(N)=-ALPHB3(N)-(1.-CRNI)*((1./DDX**2-ALPHP1(N)/(2.*DDX))*TSP(N-1)	C	82
	1+(ALPHP2(N)-2./DDX**2-ALPHB4(N)/(DT*(1.-CRNI))*TSP(N)+(1./DDX**2+	C	83
	2ALPHP1(N)/(2.*DDX))*TSP(N+1))	C	84
	GO TO 7	C	85
6	DDX=DXP	C	86
	AS(N)=CRNI*(ALPHA1(N)*DXP/(DXP1*(DXP+DXP1))-2./(DXP1*(DXP+DXP1)))	C	87
	BS(N)=CRNI*(2./(DXP*DXP1)-ALPHA2(N)-ALPHA1(N)*(DXP-DXP1)/(DXP1*DXP	C	88
	1))-ALPHB4(N)/DT	C	89
	CS(N)=CRNI*(-2./(DXP*(DXP1+DXP))-ALPHA1(N)*DXP1/(DXP*(DXP1+DXP)))	C	90
	DS(N)=-ALPHB3(N)-(1.-CRNI)*(ALPHP1(N)*DXP/(DXP1*(DXP1+DXP))-2./(DX	C	91
	1P1*(DXP1+DXP))*TSP(N-1)-((1.-CRNI)*(2./(DXP*DXP1)-ALPHP2(N)-ALPHP	C	92
	21(N)*(DXP-DXP1)/(DXP1*DXP))+ALPHB4(N)/DT)*TSP(N)+(1.-CRNI)*(2./(DX	C	93
	3P*(DXP1+DXP))+ALPHP1(N)*DXP1/(DXP*(DXP1+DXP))*TSP(N+1)	C	94
7	CONTINUE	C	95
	IF (IOPT1.EQ.0) GO TO 8	C	96
	IF ((FS(I)-TIBAR).GT.1.E-6) GO TO 9	C	97
8	CONTINUE	C	98
	AKSL=DX*KS(I)*ALPHI4/L	C	99
	AKPL=DXP1*KP(I)*GAMMI4/LP	C	100
	AKAL=CRNI/(AKSL+AKPL)	C	101
	AKSLP=DX*KSPI*ALPHIP4/LPP	C	102
	AKPLP=DXP1*KPPI*GAMMIP4/LPPP	C	103
	AKALP=(1.-CRNI)/(AKSLP+AKPLP)	C	104
	ZIS=-AKAL*KS(I)/(6.*DX*L)	C	105

YIS=AKAL*KS(I)/L*(.75/DX+ALPHI1/3.)	C 106
XIS=-AKAL*KS(I)/L*(4./(3.*DX)+1.5*ALPHI1)	C 107
AIS=-AKAL*KS(I)/L*(.75/DX-3.*ALPHI1)	C 108
BIS=AKAL*(KS(I)/L*(1.5/DX-11.*ALPHI1/6.-ALPHI2*DX)+KP(I)/LP*(1.5/D	C 109
1XP1+11.*GAMMI1/6.-GAMMI2*DXP1))-1./DT	C 110
CIS=-AKAL*KP(I)/LP*(.75/DXP1+3.*GAMMI1)	C 111
EIS=-AKAL*KP(I)/LP*(4./(3.*DXP1)-1.5*GAMMI1)	C 112
FIS=AKAL*KP(I)/LP*(.75/DXP1-GAMMI1/3.)	C 113
GIS=-AKAL*KP(I)/(LP*DXP1*6.)	C 114
DIS=-11.*AKAL/6.*(MGDOT*DHP-6.*ALPHI3/11.*DX*KS(I)/L-6.*GAMMI3*DXP	C 115
11*KP(I)/(11.*LP))-11.*AKALP/6.*(MGDOTP*DHP-6.*ALPHIP3*DX*KSPI/(11.	C 116
2*LPP)-6.*GAMMIP3*DXP1*KPPI/(LPPP*11.))+AKALP*KSPI/LPP*(TSP(I-4)/(6	C 117
3.*DX)-(.75/DX+ALPHIP1/3.)*TSP(I-3)+(4./(3.*DX)+1.5*ALPHIP1)*TSP(I-	C 118
42)+(.75/DX-3.*ALPHIP1)*TSP(I-1))-(AKALP*(KSPI/LPP*(1.5/DX-11.*ALPH	C 119
5IP1/6.-ALPHIP2*DX)+KPPI/LPPP*(1.5/DXP1+11.*GAMMIP1/6.-GAMMIP2*DXP1	C 120
6))+1./DT)*TSP(I)+AKALP*KPPI/LPPP*(.75/DXP1+3.*GAMMIP1)*TSP(I+1)+(	C 121
74./(3.*DXP1)-1.5*GAMMIP1)*TSP(I+2)-(.75/DXP1-GAMMIP1/3.)*TSP(I+3)+	C 122
8TSP(I+4)/(6.*DXP1))	C 123
AS(I)=-((BS(I-1)*XIS/AS(I-1)-CS(I-3)*BS(I-1)*ZIS/(AS(I-1)*AS(I-3))-	C 124
1BS(I-1)*BS(I-2)*YIS/(AS(I-1)*AS(I-2))+BS(I-1)*BS(I-2)*BS(I-3)*ZIS/	C 125
2(AS(I-1)*AS(I-2)*AS(I-3))-AIS+CS(I-2)*YIS/AS(I-2)-BS(I-3)*CS(I-2)*	C 126
3ZIS/(AS(I-2)*AS(I-3)))	C 127
BS(I)=-((-BIS+AS(I+1)*EIS/CS(I+1)-AS(I+1)*AS(I+3)*GIS/(CS(I+3)*CS(I	C 128
1+1))-AS(I+1)*BS(I+2)*FIS/(CS(I+1)*CS(I+2))+AS(I+1)*BS(I+2)*BS(I+3)	C 129
2*GIS/(CS(I+1)*CS(I+2)*CS(I+3))+CS(I-1)*XIS/AS(I-1)-CS(I-1)*CS(I-3)	C 130
3*ZIS/(AS(I-1)*AS(I-3))-BS(I-2)*CS(I-1)*YIS/(AS(I-1)*AS(I-2))+BS(I-	C 131
42)*BS(I-3)*CS(I-1)*ZIS/(AS(I-1)*AS(I-2)*AS(I-3)))	C 132
CS(I)=-BS(I+1)*EIS/CS(I+1)+AS(I+3)*BS(I+1)*GIS/(CS(I+1)*CS(I+3))+B	C 133
1S(I+1)*BS(I+2)*FIS/(CS(I+1)*CS(I+2))-BS(I+1)*BS(I+2)*BS(I+3)*GIS/(	C 134
2CS(I+1)*CS(I+2)*CS(I+3))+CIS-AS(I+2)*FIS/CS(I+2)+AS(I+2)*BS(I+3)*G	C 135
3IS/(CS(I+2)*CS(I+3))	C 136
DS(I)=-DS(I+1)*EIS/CS(I+1)+AS(I+3)*DS(I+1)*GIS/(CS(I+1)*CS(I+3))+B	C 137
1S(I+2)*DS(I+1)*FIS/(CS(I+1)*CS(I+2))-BS(I+2)*BS(I+3)*DS(I+1)*GIS/(	C 138
2CS(I+1)*CS(I+2)*CS(I+3))+DIS-DS(I+3)*GIS/CS(I+3)-DS(I+2)*FIS/CS(I+	C 139
33)+BS(I+3)*DS(I+2)*GIS/(CS(I+2)*CS(I+3))+DS(I-1)*CS(I-3)*ZIS/(AS(I	C 140
4-1)*AS(I-3))+BS(I-2)*DS(I-1)*YIS/(AS(I-1)*AS(I-2))-BS(I-2)*BS(I-3)	C 141



	5*DS(I-1)*ZIS/(AS(I-1)*AS(I-2)*AS(I-3))-DS(I-3)*ZIS/AS(I-3)-DS(I-2)	C 142
	6*YIS/AS(I-2)+BS(I-3)*DS(I-2)*ZIS/(AS(I-2)*AS(I-3))-DS(I-1)*XIS/AS(I-1)	C 143
	7I-1)	C 144
	GO TO 10	C 145
9	CONTINUE	C 146
	AS(I)=0.	C 147
	BS(I)=1.	C 148
	CS(I)=0.	C 149
	DS(I)=TIBAR+1.E-4	C 150
10	CONTINUE	C 151
	DO 11 N=IP1, IZ1	C 152
	AS(N)=CRNI*(1./DXPP**2-ALPHA1(N)/(2.*DXPP))	C 153
	BS(N)=CRNI*(ALPHA2(N)-2./DXPP**2+ALPHA4(N)/(DT*CRNI))	C 154
	CS(N)=CRNI*(1./DXPP**2+ALPHA1(N)/(2.*DXPP))	C 155
	DS(N)=-ALPHA3(N)-(1.-CRNI)*((1./DXPP**2-ALPHA1(N)/(2.*DXPP))*TSP(N	C 156
	1-1)+(ALPHA2(N)-2./DXPP**2-ALPHA4(N)/(DT*(1.-CRNI)))*TSP(N)+(1./DXP	C 157
	2P**2+ALPHA1(N)/(2.*DXPP))*TSP(N+1))	C 158
11	CONTINUE	C 159
	AK=CRNI/(KP(IP)*GAMIP4*DXP/LP+KPP(IP)*KAPIP4*DXPP/IL-HTSK)	C 160
	AKP=(1.-CRNI)/(KPPIP*GAMIPP4*DXP/LPPP+KPPPIP*KAPIPP4*DXPP/IL-HTSK)	C 161
	ZIS=-AK*KP(IP)/(6.*DXP*LP)	C 162
	YIS=AK*KP(IP)*(0.75/DXP+GAMIP1/3.)/LP	C 163
	XIS=-AK*KP(IP)*(4./(3.*DXP)+1.5*GAMIP1)/LP	C 164
	AIS=-AK*KP(IP)*(0.75/DXP-3.*GAMIP1)/LP	C 165
	BIS=-1./DT+AK*(KP(IP)/LP*(1.5/DXP-11.*GAMIP1/6.-GAMIP2*DXP)+KPP(IP	C 166
	1)/IL*(1.5/DXPP+11.*KAPIP1/6.-KAPIP2*DXPP))	C 167
	CIS=-AK*KPP(IP)*(0.75/DXPP+3.*KAPIP1)/IL	C 168
	EIS=-AK*KPP(IP)*(4./(3.*DXPP)-1.5*KAPIP1)/IL	C 169
	FIS=AK*KPP(IP)*(0.75/DXPP-KAPIP1/3.)/IL	C 170
	GIS=-AK*KPP(IP)/(6.*DXPP*IL)	C 171
	DIS=AK*(KP(IP)*GAMIP3*DXP/LP+KPP(IP)*KAPIP3*DXPP/IL)-AKP*KPPIP/LPP	C 172
	IP*(-TSP(IP-4)/(6.*DXP)+(0.75/DXP+GAMIP1/3.)*TSP(IP-3)-(4./(3.*DXP)	C 173
	2+1.5*GAMIPP1)*TSP(IP-2)-(0.75/DXP-3.*GAMIPP1)*TSP(IP-1))-(AKP*(KPPI	C 174
	3P/LPPP*(1.5/DXP-11.*GAMIPP1/6.-GAMIPP2*DXP)+KPPPIP/IL*(1.5/DXPP+11	C 175
	4.*KAPIPP1/6.-KAPIPP2*DXPP))+1./DT)*TSP(IP)+AKP*KPPPIP/IL*((0.75/DXP	C 176

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5P+3.*KAPIPP1)*TSP(IP+1)+(4./(3.*DXPP)-1.5*KAPIPP1)*TSP(IP+2)-(.75/ C 177
6DXPP-KAPIPP1/3.)*TSP(IP+3)+TSP(IP+4)/(6.*DXPP))+AKP*(KPPIP*GAMIPP3 C 178
7*DXP/LPPP+KPPPIP*KAPIPP3*DXPP/IL) C 179
AS(IP)=-(BS(IP-1)*XIS/AS(IP-1)-CS(IP-3)*BS(IP-1)*ZIS/(AS(IP-1)*AS( C 180
1IP-3))-BS(IP-1)*BS(IP-2)*YIS/(AS(IP-1)*AS(IP-2))+BS(IP-1)*BS(IP-2) C 181
2*BS(IP-3)*ZIS/(AS(IP-1)*AS(IP-2)*AS(IP-3))-AIS+CS(IP-2)*YIS/AS(IP- C 182
32)-BS(IP-3)*CS(IP-2)*ZIS/(AS(IP-2)*AS(IP-3))) C 183
BS(IP)=-(-BIS+AS(IP+1)*EIS/CS(IP+1)-AS(IP+1)*AS(IP+3)*GIS/(CS(IP+3 C 184
1)*CS(IP+1))-AS(IP+1)*BS(IP+2)*FIS/(CS(IP+1)*CS(IP+2))+AS(IP+1)*BS( C 185
2IP+2)*BS(IP+3)*GIS/(CS(IP+1)*CS(IP+2)*CS(IP+3))+CS(IP-1)*XIS/AS(IP C 186
3-1)-CS(IP-1)*CS(IP-3)*ZIS/(AS(IP-1)*AS(IP-3))-BS(IP-2)*CS(IP-1)*YI C 187
4S/(AS(IP-1)*AS(IP-2))+BS(IP-2)*BS(IP-3)*CS(IP-1)*ZIS/(AS(IP-1)*AS( C 188
5IP-2)*AS(IP-3))) C 189
CS(IP)=-3S(IP+1)*EIS/CS(IP+1)+AS(IP+3)*BS(IP+1)*GIS/(CS(IP+1)*CS(I C 190
1P+3))+BS(IP+1)*BS(IP+2)*FIS/(CS(IP+1)*CS(IP+2))-BS(IP+1)*BS(IP+2)* C 191
2BS(IP+3)*GIS/(CS(IP+1)*CS(IP+2)*CS(IP+3))+CIS-AS(IP+2)*FIS/CS(IP+2 C 192
3)+AS(IP+2)*BS(IP+3)*GIS/(CS(IP+2)*CS(IP+3)) C 193
DS(IP)=-DS(IP+1)*EIS/CS(IP+1)+AS(IP+3)*DS(IP+1)*GIS/(CS(IP+1)*CS(I C 194
1P+3))+BS(IP+2)*DS(IP+1)*FIS/(CS(IP+1)*CS(IP+2))-BS(IP+2)*BS(IP+3)* C 195
2DS(IP+1)*GIS/(CS(IP+1)*CS(IP+2)*CS(IP+3))+DIS-DS(IP+3)*GIS/CS(IP+3 C 196
3)-DS(IP+2)*FIS/CS(IP+3)+BS(IP+3)*DS(IP+2)*GIS/(CS(IP+2)*CS(IP+3))+ C 197
4DS(IP-1)*CS(IP-3)*ZIS/(AS(IP-1)*AS(IP-3))+BS(IP-2)*DS(IP-1)*YIS/(A C 198
5S(IP-1)*AS(IP-2))-BS(IP-2)*BS(IP-3)*JS(IP-1)*ZIS/(AS(IP-1)*AS(IP-2 C 199
6)*AS(IP-3))-DS(IP-3)*ZIS/AS(IP-3)-DS(IP-2)*YIS/AS(IP-2)+BS(IP-3)*D C 200
7S(IP-2)*ZIS/(AS(IP-2)*AS(IP-3))-DS(IP-1)*XIS/AS(IP-1) C 201
ZSCNST=CRNI*KPP(IZ)/(6.*DXPP**2*IL*(HTSKP*(ALPHA1(IZ)+11./(6.*DXPP C 202
1))-ALPHA4(IZ)*KPP(IZ)/IL)) C 203
YSCNST=-4.5*ZSCNST C 204
XSCNST=8.*ZSCNST C 205
AS(IZ)=-YSCNST C 206
BS(IZ)=(6.*DXPP**2*ALPHA2(IZ)-9.)*ZSCNST-CRNI*SGMA*EPSP*FS(IZ)**3* C 207
1(ALPHA1(IZ)+11./(6.*DXPP))/(HTSKP*(ALPHA1(IZ)+11./(6.*DXPP))-ALPHA C 208
24(IZ)*KPP(IZ)/IL)-1./DT C 209
DS(IZ)=-CRNI*(ALPHA1(IZ)+11./(6.*DXPP))/(HTSKP*(ALPHA1(IZ)+11./(6. C 210
1*DXPP))-ALPHA4(IZ)*KPP(IZ)/IL)*(GNET+ALPHA3(IZ)*KPP(IZ)/(IL*(ALPHA C 211

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	21(IZ)+11./(6.*DXPP))))-(1.-CRNI)*(ALPHP1(IZ)+11./(6.*DXPP))/(HTSKP	C 212
	3*(ALPHP1(IZ)+11./(6.*DXPP))-ALPHP4(IZ)*KPPP IZ/IL)*(QNET+ALPHP3(IZ	C 213
	4)*KPPP IZ/(IL*(ALPHP1(IZ)+11./(6.*DXPP)))+KPPP IZ/(IL*(ALPHP1(IZ)+11	C 214
	5./(6.*DXPP))*(TSP(IZ-4)/(6.*DXPP**2)-.75*TSP(IZ-3)/DXPP**2+.75*TSP	C 215
	6(IZ-2)/(3.*DXPP**2)+.75*TSP(IZ-1)/DXPP**2-(1.5/DXPP**2-ALPHP2(IZ))	C 216
	7*TSP(IZ))-SGMA*EPSP*TSP(IZ)**4)-TSP(IZ)/DT	C 217
	AS(IZ)=AS(IZ-2)*BS(IZ-1)*(AS(IZ-3)*XSCNST-CS(IZ-3)*ZSCNST)-BS(IZ-1	C 218
	1)*BS(IZ-2)*(AS(IZ-3)*YSCNST-BS(IZ-3)*ZSCNST)+AS(IZ-1)*CS(IZ-2)*(AS	C 219
	2(IZ-3)*YSCNST-BS(IZ-3)*ZSCNST)-AS(IZ)*AS(IZ-1)*AS(IZ-2)*AS(IZ-3)	C 220
	BS(IZ)=AS(IZ-2)*CS(IZ-1)*(AS(IZ-3)*XSCNST-CS(IZ-3)*ZSCNST)-BS(IZ-2	C 221
	1)*CS(IZ-1)*(AS(IZ-3)*YSCNST-BS(IZ-3)*ZSCNST)-AS(IZ-1)*AS(IZ-2)*AS(I	C 222
	2IZ-3)*BS(IZ)	C 223
	DS(IZ)=AS(IZ-2)*DS(IZ-1)*(AS(IZ-3)*XSCNST-CS(IZ-3)*ZSCNST)-BS(IZ-2	C 224
	1)*DS(IZ-1)*(AS(IZ-3)*YSCNST-BS(IZ-3)*ZSCNST)-AS(IZ-1)*AS(IZ-2)*(AS	C 225
	2(IZ-3)*DS(IZ)-DS(IZ-3)*ZSCNST)+AS(IZ-1)*DS(IZ-2)*(AS(IZ-3)*YSCNST-	C 226
	3BS(IZ-3)*ZSCNST)	C 227
	CS(IZ)=0.	C 228
C	SOLVE TRI-DIAGONAL MATRIX FOR TS	C 229
	BP(1)=CS(1)/BS(1)	C 230
	GP(1)=DS(1)/BS(1)	C 231
	DO 12 N=2, IZ	C 232
	WS=BS(N)-AS(N)*BP(N-1)	C 233
	BP(N)=CS(N)/WS	C 234
	GP(N)=(DS(N)-AS(N)*GP(N-1))/WS	C 235
12	CONTINUE	C 236
	TFS(IZ)=GP(IZ)	C 237
	FS(IZ)=TFS(IZ)	C 238
	KON=IZ1	C 239
	DO 13 N=1, IZ1	C 240
	TFS(KON)=GP(KON)-BP(KON)*TFS(KON+1)	C 241
	FS(KON)=TFS(KON)	C 242
13	KON=KON-1	C 243
	RETURN	C 244
	END	C 245-

	SUBROUTINE PDP (CRNI,DT,L,DX,DX1,MGDOT,MGDOTP,LPP,I,IM,RHO,P,MU,T,	D	1
	1TP,RU)	D	2
C	SUBROUTINE FOR SOLVING SECOND ORDER LINEARIZED DIFFERENTIAL EQUA-	D	3
C	TIONS FOR PYROLYSIS GAS PRESSURE IN THE CHAR LAYER.	D	4
	DIMENSION RHO(50), P(50), MU(50), AS(50), BS(50), CS(50), DS(50),	D	5
	1BP(50), GP(50), T(50), TP(50), ZP(50)	D	6
	COMMON /PDP/ PAL1(50),PAL2(50),PAL3(50),PAL4(50),PAP1(50),PAP2(50)	D	7
	1,PAP3(50),PAP4(50),PAB3(50),PAB4(50),PWP,PP(50),PM(50),PMU,PPM,PRH	D	8
	20(50),ETA(50),ETAP(50),AVGMF(50),AVGMFP(50)	D	9
	COMMON /DE1DE2/ AS,BS,CS,DS,BP,GP	D	10
	REAL MU,L,MGDOT,LPP,MGDOTP	D	11
	DOUBLE PRECISION AS,BS,CS,DS,PX,PY,PZ,PA,PB,PD,BP,GP,W,ZP	D	12
C	CALCULATE TRI-DIAGONAL MATRIX COEFFICIENTS	D	13
	IN=I-2	D	14
	DDX=DX1	D	15
	DO 2 N=2,IM	D	16
	IF (N.NE.20) GO TO 1	D	17
	DDX=DX	D	18
	GO TO 2	D	19
1	AS(N)=CRNI*(1./DDX**2-PAL1(N)/(2.*DDX))	D	20
	BS(N)=CRNI*(PAL2(N)-2./DDX**2)+PAB4(N)/DT	D	21
	CS(N)=CRNI*(1./DDX**2+PAL1(N)/(2.*DDX))	D	22
	DS(N)=-PAB3(N)-(1.-CRNI)*((1./DDX**2-PAP1(N)/(2.*DDX))*PP(N-1)**2-	D	23
	1(2./DDX**2-PAP2(N)+PAB4(N)/(DT*(1.-CRNI)))*PP(N)**2+(1./DDX**2+PAP	D	24
	21(N)/(2.*DDX))*PP(N+1)**2)	D	25
2	CONTINUE	D	26
	AS(20)=CRNI*(PAL1(20)*DX/(DX1*(DX1+DX))-2./(DX1*(DX1+DX)))	D	27
	BS(20)=CRNI*(2./(DX*DX1)-PAL2(20)-PAL1(20)*(DX-DX1)/(DX1*DX))-PAB4	D	28
	1(20)/DT	D	29
	CS(20)=CRNI*(-2./(DX*(DX1+DX))-PAL1(20)*DX1/(DX*(DX1+DX)))	D	30
	DS(20)=-PAB3(20)-(1.-CRNI)*(PAP1(20)*DX/(DX1*(DX1+DX))-2./(DX1*(DX	D	31
	11+DX))*PP(19)**2-((1.-CRNI)*(2./(DX*DX1)-PAP2(20)-PAP1(20)*(DX-DX	D	32
	21)/(DX1*DX))+PAB4(20)/DT)*PP(20)**2+(1.-CRNI)*(2./(DX*(DX1+DX))+PA	D	33
	3P1(20)*DX1/(DX*(DX1+DX))*PP(21)**2	D	34
	DS(2)=DS(2)-AS(2)*P(1)**2	D	35
	AS(2)=0.	D	36

	PX=CRNI/(6.*DX**2)	D	37
	PY=-.75*CRNI/DX**2	D	38
	PZ=4.*CRNI/(3.*DX**2)	D	39
	PA=-PY	D	40
	PB=PAB4(I)/DT+CRNI*(PAL2(I)-3./(2.*DX**2))	D	41
	PD=-PAB3(I)-(1.-CRNI)*(11./(6.*DX)+PAP1(I))*(2.*PMU*LPP*MGDOTP*RU*	D	42
	1TP(I)/(AVGMFP(I)*PPM))-CRNI*(11./(6.*DX)+PAL1(I))*(2.*MU(I)*L*MGDO	D	43
	2T*RU*T(I)/(AVGMF(I)*PM(I))-(1.-CRNI)*(PP(I-4)**2/(6.*DX**2)-.75*P	D	44
	3P(I-3)**2/DX**2+4.*PP(I-2)**2/(3.*DX**2)+.75*PP(I-1)**2/DX**2+(PAP	D	45
	42(I)-1.5/DX**2-PAB4(I)/(DT*(1.-CRNI)))*PP(I)**2)	D	46
	AS(I)=PA-CS(I-2)/AS(I-2)*(PY-PX*BS(I-3)/AS(I-3))-BS(I-1)/AS(I-1)*(	D	47
	1PZ-PX*CS(I-3)/AS(I-3)-BS(I-2)/AS(I-2)*(PY-PX*BS(I-3)/AS(I-3)))	D	48
	BS(I)=PB-CS(I-1)/AS(I-1)*(PZ-PX*CS(I-3)/AS(I-3)-BS(I-2)/AS(I-2)*(P	D	49
	1Y-PX*BS(I-3)/AS(I-3)))	D	50
	DS(I)=PD-PX/AS(I-3)*DS(I-3)-DS(I-2)/AS(I-2)*(PY-PX*BS(I-3)/AS(I-3)	D	51
	1)-DS(I-1)/AS(I-1)*(PZ-PX*CS(I-3)/AS(I-3)-BS(I-2)/AS(I-2)*(PY-PX*BS	D	52
	2(I-3)/AS(I-3)))	D	53
	CS(I)=0.	D	54
C	SOLVE TRI-DIAGONAL MATRIX FOR P	D	55
	BP(2)=CS(2)/BS(2)	D	56
	GP(2)=DS(2)/BS(2)	D	57
	DO 3 N=3,I	D	58
	W=BS(N)-AS(N)*BP(N-1)	D	59
	BP(N)=CS(N)/W	D	60
	GP(N)=(DS(N)-AS(N)*GP(N-1))/W	D	61
3	CONTINUE	D	62
	ZP(I)=DSQRT(GP(I))	D	63
	P(I)=ZP(I)	D	64
	KON=IM	D	65
	DO 4 N=1,IN	D	66
	ZP(KON)=DSQRT(GP(KON)-BP(KON)*ZP(KON+1)**2)	D	67
	P(KON)=ZP(KON)	D	68
4	KON=KON-1	D	69
	RETURN	D	70
	END	D	71-

	SUBROUTINE PDF2 (BETA1,BETB2,BETB3,BETP1,TP,F,CRNI,DX,DX1,DT,I)	E	1
C	SUBROUTINE FOR SOLVING FIRST ORDER LINEARIZED DIFFERENTIAL	E	2
C	EQUATIONS GOVERNING PYROLYSIS GAS TEMPERATURE AND FLOW RATE AND	E	3
C	CHAR LAYER POROSITY.	E	4
	DIMENSION B(50), C(50), D(50), E(50), F(50), TP(50), BETA1(50), BE	E	5
	1TB2(50), BETB3(50), BETP1(50), TF(50)	E	6
	COMMON /DE1DE2/ B,C,D,E	E	7
	DOUBLE PRECISION B,C,D,E,TF	E	8
C	CALCULATE TRI-DIAGCNAL MATRIX COEFFICIENTS	E	9
	IM=I-1	E	10
	IN=I-2	E	11
	IQ=I-3	E	12
	DDX=DX1	E	13
	B(19)=BETB3(19)/DT+CRNI*(-(DX**2+2.*DX1*DX)/(DX1*DX*(DX1+DX))+BETA	E	14
	11(19))	E	15
	C(19)=CRNI*(DX1+DX)/(DX1*DX)	E	16
	E(19)=-CRNI*DX1/(DX*(DX1+DX))	E	17
	D(19)=-BETB2(19)+(BETB3(19)/DT-(1.-CRNI)*(-(DX**2+2.*DX1*DX)/(DX1*	E	18
	1DX*(DX1+DX))+BETP1(19))*TP(19)-(1.-CRNI)*(DX1+DX)/(DX1*DX)*TP(20)	E	19
	2+(1.-CRNI)*DX1/(DX*(DX1+DX))*TP(21)	E	20
	DO 2 N=1,IN	E	21
	IF (N.NE.19) GO TO 1	E	22
	DDX=DX	E	23
	GO TO 2	E	24
1	CONTINUE	E	25
	B(N)=CRNI*(BETA1(N)-1.5/DDX)+BETB3(N)/DT	E	26
	C(N)=2.*CRNI/DDX	E	27
	E(N)=-.5*CRNI/DDX	E	28
	D(N)=-BETB2(N)-((1.-CRNI)*(BETP1(N)-1.5/DDX)-BETB3(N)/DT)*TP(N)-(1	E	29
	1.-CRNI)*(2.*TP(N+1)/DDX-TP(N+2)/(2.*DDX))	E	30
2	CONTINUE	E	31
	B(IM)=CRNI*(BETA1(IM)-1./DX)+BETB3(IM)/DT	E	32
	C(IM)=CRNI/DX	E	33
	E(IM)=0.	E	34
	D(IM)=-BETB2(IM)-((1.-CRNI)*(BETP1(IM)-1./DX)-BETB3(IM)/DT)*TP(IM)	E	35
	1-(1.-CRNI)/DX*TP(I)	E	36

C	SOLVE TRI-DIAGONAL MATRIX	E	37
	TF(I)=F(I)	E	38
	TF(IM)=(D(IM)-C(IM)*TF(I))/B(IM)	E	39
	F(IM)=TF(IM)	E	40
	KON=IN	E	41
	DO 3 N=1,IN	E	42
	TF(KON)=(D(KON)-C(KON)*TF(KON+1)-E(KON)*TF(KON+2))/B(KON)	E	43
	F(KON)=TF(KON)	E	44
3	KON=KON-1	E	45
	RETURN	E	46
	END	E	47-

	SUBROUTINE CHCOM(TIME)	F	1
C	SUBROUTINE FOR CALCULATING THE CHEMICAL REACTION RATES OF EACH	F	2
C	SPECIES.	F	3
	COMMON ACEF(12),ACER(12),BCEF(12),BCER(12),CRNI,KUPT(40,12),KUPTV(		4
	140),M(13),MFK(50,12),MNO,NNO,MU(50),MUKT(40,12),MUKTV(40),PR(50),R	F	5
	2(50,12),RHO(50),RHOK(50,12),RHOKP(50,12),T(50),TEMP(40),NRCT,KT,RU	F	6
	3,NSTEP,RDCPM(50),RS(50),RHR(50,12),RHS(50),DHK(50,12),DHJ(50,12),H	F	7
	4RJSUM(50)	F	8
	DIMENSION RMP(9),RMR(9),RJN(9)	F	9
	REAL M	F	10
	N=NSTEP	F	11
	RMR(1)=RHCK(N,1)/M(1)	F	12
	RMP(1)=1.	F	13
	RMR(2)=RHOK(N,11)/M(11)	F	14
	RMP(2)=RHOK(N,3)/M(3)*RHOK(N,2)/M(2)	F	15
	RMR(3)=RHOK(N,3)/M(3)	F	16
	RMP(3)=RHOK(N,4)/M(4)*RHOK(N,2)/M(2)	F	17
	RMR(4)=(RHOK(N,4)/M(4))**2	F	18
	RMP(4)=1.	F	19
	RMR(5)=RHOK(N,12)/M(12)	F	20
	RMP(5)=1.	F	21
	RMR(6)=RHOK(N,9)/M(9)	F	22
	RMP(6)=1.	F	23
	RMR(7)=RHCK(N,6)/M(6)	F	24
	RMP(7)=1.	F	25
	RMR(8)=RHOK(N,7)/M(7)	F	26
	RMP(8)=1.	F	27
	RMR(9)=RHOK(N,7)/M(7)	F	28
	RMP(9)=1.	F	29
	DO 1 J=1,9	F	30
	AKF=ACEF(J)*EXP(-BCEF(J)/(RU*T(N)))	F	31
	IF(J.EQ.6)AKF=AKF/T(N)	F	32
	AKK=ACER(J)*EXP(-BCER(J)/(RU*T(N)))	F	33
	RJN(J)= AKF*RMR(J)-AKK*RMP(J)	F	34
1	CONTINUE	F	35
	R(N,1)=-RJN(1)	F	36



R(N,2)=.5*RJN(1)+RJN(2)+RJN(3)+RJN(4)+3.*RJN(5)+RJN(7)+1.5*RJN(8)+	F	37
1RJN(9)	F	38
R(N,3)=RJN(2)-RJN(3)	F	39
R(N,4)=RJN(3)-RJN(4)	F	40
R(N,5)=2.*RJN(6)+RJN(7)	F	41
R(N,6)=-RJN(7)	F	42
R(N,7)=-RJN(8)-RJN(9)	F	43
R(N,8)=.5*RJN(8)-RJN(9)	F	44
R(N,9)=-RJN(6)	F	45
R(N,10)=RJN(9)	F	46
R(N,11)=.5*RJN(1)-RJN(2)	F	47
R(N,12)=-RJN(5)	F	48
RS(N)=2.*RJN(4)+6.*RJN(5)	F	49
RHS(N)=-RJN(6)-RJN(7)-RJN(9)	F	50
RHR(N,6)=RJN(6)	F	51
RHR(N,7)=RJN(7)	F	52
RHR(N,9)=RJN(9)	F	53
RETURN	F	54
END	F	55-

## APPENDIX D

### PROGRAM TERMINOLOGY

A	Dummy parameter used in computing viscosity of pyrolysis gas
AB2	Dummy array defined in solution of species continuity equation, single subscript
AC	Specific reaction rate constant for first order oxidation of char layer
ACEF	Specific reaction rate constant for forward chemical reaction, single subscript
ACER	Specific reaction rate constant for reverse chemical reaction, single subscript
AEXP	Specific reaction rate constant for pyrolysis gas of uncharred material
AINT	Single subscripted parameter defined as $\int_{x(N)}^1 \eta \rho \, dx$
AINT3	Single subscripted parameter defined as $\int_{x(N)}^1 \left[ \frac{\partial}{\partial t} \eta \rho - \eta \sum_i R_{T_i} M_i \right] dx$
AIS	Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer - insulation layer interface
AISCNST	Coefficient in solid temperature finite difference equation evaluated at the front surface of the char layer
AK	Parameter defined in solution of solid temperature equation
AKAL	Parameter defined in solution of solid temperature equation
AKALP	Parameter defined in solution of solid temperature equation
AKF	Rate of homogeneous chemical reaction in forward direction, single subject

AKP	Parameter defined in solution of solid temperature equation
AKPL	Parameter defined in solution of solid temperature equation
AKPLP	Parameter defined in solution of solid temperature equation
AKR	Rate of homogeneous chemical reaction in reverse direction, single subscript
AKSL	Parameter defined in solution of solid temperature equation
AKSLP	Parameter defined in solution of solid temperature equation
ALFC	Weighting factor for transpiration effectiveness of char mass loss
ALFP	Weighting factor for transpiration effectiveness of pyrolysis gases
ALPHA	Absorptivity of char surface
ALPHA 1 ALPHA 2 ALPHA 3 ALPHA 4	Coefficients in linearized differential equations for solid temperature evaluated at end of time step, single subscript
ALPHB3 ALPHB4	Coefficients in finite difference equation for solid temperature evaluated at mid point of time step, single subscript
ALPHIP1 ALPHIP2 ALPHIP3 ALPHIP4	Values of ALPHA1, etc. for the char layer at the pyrolysis zone evaluated at the start of the time step
ALPHI1 ALPHI2 ALPHI3 ALPHI4	Values of ALPHA1, etc. for the char layer at the pyrolysis zone evaluated at the end of the time step
ALPHP1 ALPHP2 ALPHP3 ALPHP4	Values of ALPHA1, etc. evaluated at the start of the time step, single subscript

ALI	Dummy array defined in solving species continuity equation, single subscript
AMDOT	Local mass flow rate of pyrolysis gas, single subscript
AMGDOT	Rate of pyrolysis of uncharred material given by rate equation
AMSDOT	Rate of char layer removed by oxidation
AMU AMJ	} Dummy parameter defined in computing pyrolysis gas viscosity
AP	
APR	Dummy parameter defined in computing pyrolysis gas Prandtl number
AP1 ARH	} Dummy arrays defined in solution of species continuity equation, single subscript
AS	
AT	Pyrolysis gas temperature for previous iteration, single subscript
ATS	Solid temperature for previous iteration, single subscript
AVGMF	Average molecular weight of pyrolysis gas at end of time step, double subscript
AVGMFP	Average molecular weight of pyrolysis gas at start of time step, double subscript
B	"B" coefficient in matrix formed by first order equations, single subscript
BC	Activation temperature for first order oxidation of char layer
BCEF	Activation temperature for forward homogeneous chemical reaction involving gaseous species, single subject
BCER	Activation temperature for reverse homogeneous chemical reaction involving gaseous species, single subscript

BETA1 BETA2 BETA3	} Coefficients in linearized differential equation of pyrolysis gas temperature evaluated at end of time step, single subscript
BETB2 BETB3	} Coefficients in finite difference equation for pyrolysis gas temperature evaluated at mid point of time step, single subscript
BETP1 BETP2 BETP3	} Values of BETA1, etc. evaluated at the start of the time step, single subscript
BEXP	Activation temperature for pyrolysis of uncharred material
BIS	Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer-insulation layer.
BMGDOT	Rate of pyrolysis of uncharred material given by energy-balance
BMSDOT	Rate of removal of char layer by sublimation
BP	Parameter defined in algorithm for solving set of finite difference equations, single subscript
BRH	Dummy array defined in solution of species continuity equation, single subscript
BS	"BS" coefficient in matrix formed by second order differential equation, single subscript
C	"C" coefficient in matrix formed by first order equations, single subscript
CE	Mass fraction of oxygen at edge of boundary layer
CIS	Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer-insulation layer interface
CPK	Heat capacity of gaseous species, double subscript
CPKT	Table of gaseous species heat capacity versus temperature, double subscript
CPKTV	Dummy array defined for use in table-look-up routine to obtain CPK, single subscript

CPP	Heat capacity of uncharred material, single subscript
CPPP	Heat capacity of insulation layer, single subscript
CPPPV	Constant heat capacity of insulation layer
CPPT	Table of uncharred material heat capacity versus temperature, single subscript
CPS	Heat capacity of char layer, single subscript
CPSA11 } CPSA12 }	Dummy parameters defined in computing CPK
CPSV	Constant heat capacity of char layer
CRNI	Crank-Nicolson factor - $1/2$ for modified implicit solution
CS	"CS" coefficient in matrix formed by second order differential equation, single subscript
D	"D" coefficient in matrix formed by first order differential equations, single subscript
DDX	Distance between finite difference stations
DEB2 } DEB3 }	Coefficients in finite difference equation for conservation of species evaluated at mid point of time step, single subscript
DEL1 } DEL2 } DEL3 }	Coefficients in linearized differential equation for conservation of species evaluated at end of time step, double subscript
DEN	Denominator defined in solution of first order equations
DEP1 } DEP2 } DEP3 }	Values of DEL1, etc. evaluated at start of time step, double subscript
DETADX	Porosity gradient in char layer, single subscript
DHC	Heat of combustion of char layer
DHJ	Heat of reaction for heterogeneous chemical reaction, double subscript

DHK	Enthalpy of chemical species evaluated at solid temperature, double subscript
DHP	Heat of pyrolysis of uncharred material
DIFER	Convergence criteria
DIS	Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer-insulation layer interface
DKPDX	Gradient of uncharred material thermal conductivity, single subscript
DKSDX	Gradient of char layer thermal conductivity, single subscript
DL	Change in thickness of char layer
DLP	Change in thickness of uncharred layer
DMBRDX	Gradient of pyrolysis gas molecular weight, single subscript
DRHO	Difference in density of uncharred material and density of char layer at the pyrolysis zone
DRODX	Gradient of pyrolysis gas density at end of time step, single subscript
DS	"DS" coefficient in matrix formed by second order differential equation, single subscript
DT	Time increment
DTDx	Gradient of pyrolysis gas temperature at end of time step, single subscript
DVDX	Gradient of pyrolysis gas velocity, single subscript
DX	Distance between finite difference stations in char layer in region of course grid spacing
DXP	Distance between finite difference stations in uncharred layer in region of course grid spacing
DXPP	Distance between finite difference stations in insulation layer

DXP1	Distance between finite difference stations in uncharred layer in region of the fine grid spacing
DX1	Distance between finite difference stations in char layer in region of fine grid spacing
E	"E" coefficient in matrix formed by first order equations, single subscript
EIS	Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer - insulation layer interface
EPSA1 EPSA2 EPSA3	Coefficients in linearized differential equation for char layer porosity evaluated at end of time step, single subscript
EPSP1 EPSP2 EPSP3	
EPSP1 EPSP2 EPSP3	
EPSP	Emissivity of radiating heat sink surface behind insulation
EPSP1 EPSP2 EPSP3	Values of EPSA1, etc. evaluated at the start of the time step, single subscript
EPSP1 EPSP2 EPSP3	
EPSP1 EPSP2 EPSP3	
EPSS	Emissivity of char layer surface
ETA	Porosity of char layer at end of time step, single subscript
ETAP	Porosity of char layer at start of time step, single subscript
F	Dummy array defined in solution of first order differential equations, single subscript
FIS	Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer insulation layer interface
FS	Dummy array defined in solution of solid temperature equations, single subscript
GAMIPP1 GAMIPP2 GAMIPP3 GAMIPP4	Values of ALPHA1, etc. for the uncharred material at the uncharred layer-insulation layer interface evaluated at the start of the time step
GAMIPP1 GAMIPP2 GAMIPP3 GAMIPP4	
GAMIPP1 GAMIPP2 GAMIPP3 GAMIPP4	
GAMIPP1 GAMIPP2 GAMIPP3 GAMIPP4	



GAMIP1 GAMIP2 GAMIP3 GAMIP4	} Values of ALPHA1, etc. for the uncharred material at the uncharred layer-insulation layer interface evaluated at the end of the time step
GAMMI1 GAMMI2 GAMMI3 GAMMI4	} Values of ALPHA1, etc. for the uncharred material at the pyrolysis zone evaluated at the end of the time step
GIS	Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer-insulation layer interface
GP	Parameter defined in algorithm for solving set of finite difference equations, single subscript
GSCNST	Coefficient in solid temperature finite difference equation evaluated at the front surface of the char layer
HA	Coefficient of convective heat transfer between char layer and pyrolysis gas, single subscript
HBRKN2	Enthalpy of N <sub>2</sub> at char surface temperature evaluated at end of time step
HBRKO2	Enthalpy of O <sub>2</sub> at char surface temperature evaluated at end of time step
HC	Heat of sublimation of char layer material
HE	Enthalpy of free stream
HK	Enthalpy of gaseous species, double subscript
HKT	Table of gaseous species enthalpy versus temperature, double subscript
HKTV	Dummy array defined for use in table look-up routine for single subscript
HRJSUM HRSUM	} Parameters defined in computing coefficients in pyrolysis gas temperature equation, single subscript
HS	Enthalpy of char layer evaluated at the char temperature, single subscript

HSA11 } HSA12 }	Dummy parameters defined in computing HK
HSCNST	Coefficient in solid temperature finite difference equation evaluated at the front surface of the char layer
HST	Enthalpy of char layer evaluated at the pyrolysis gas temperature, single subscript
HSTT	Table of char layer enthalpy versus temperature, single subscript
HTSK	Value of $\rho \hat{C}_p l$ for heat sink at uncharred layer-insulation layer interface
HTSKP	Value of $\rho \hat{C}_p l$ for heat sink behind insulation layer
HW	Enthalpy of air at char surface temperature
I	Number of finite difference stations in the char layer
IL	Thickness of insulation layer
IM } IN } IN <sup>2</sup> } IO } IO1 }	Indices
IP	Total number of finite difference stations in char layer and uncharred material
IPP } IP1 }	Indices
IZ	Total number of finite difference stations in char layer, uncharred material, and insulation layer
IZ1 } J }	Dummy indices
JK	Number of finite difference stations in uncharred material
K	Dummy index
KA	Parameter defined in computing rate of char layer removal by first order oxidation

KAPIPP1 KAPIPP2 KAPIPP3 KAPIPP4	} Value of ALPHA1, etc. for the insulation layer at the uncharred layer-insulation layer interface evaluated at the start of the time step
KAPIP1 KAPIP2 KAPIP3 KAPIP4	} Value of ALPHA1, etc. for the insulation layer at the uncharred layer-insulation layer interface evaluated at the end of the time step
KG	Conductivity of the pyrolysis gas
KGK	Conductivity of gaseous species, single subscript
KI KM KON	} Dummy indices
KP	Conductivity of uncharred material at end of time step, single subscript
KPP	Conductivity of insulation layer, single subscript
KPPI	Conductivity of uncharred material at pyrolysis zone evaluated at start of time step
KPIIP	Conductivity of uncharred material at uncharred layer - insulation layer interface evaluated at start of time step
KPPPIP	Conductivity of insulation layer at uncharred layer-insulation layer interface evaluated at start of time step
KPPPIZ	Conductivity of insulation layer at back of insulation evaluated at start of time step
KPPV	Data input for insulation layer conductivity
KPT	Table of uncharred material conductivity versus temperature, single subscript
KS	Conductivity of char layer at end of time step, single subscript
KSPI	Conductivity of char layer at pyrolysis zone evaluated at start of time step
KSP1	Conductivity of char layer at front surface evaluated at start of time step

KST	Table of char layer conductivity versus temperature, single subscript
KT KTT	Indices
KUPT	Table of gaseous species conductivity versus temperature, double subscript
KUPTV	Dummy array defined for use in table-look-up routine for KGK, single subscript
L	Char layer thickness at end of time step
LAM	Ratio of mass char layer removed to free stream oxygen consumed in first order oxidation of char
LP	Uncharred material thickness at end of time step
LPMIN	Minimum thickness of uncharred layer
LPP	Char layer thickness at start of time step
LPPP	Uncharred material thickness at start of time step
M	Molecular weight of chemical species, single subscript
MCPP	Order of interpolation in obtaining CPP
MFK	Mole fraction of gaseous species, double subscript
MFKI	Mole fraction of gaseous species at pyrolysis zone, single subscript
MGDOT	Rate of pyrolysis of uncharred material at end of time step
MGDOTP	Rate of pyrolysis of uncharred material at start of time step
MKP	Order of interpolation in obtaining KP
MKS	Order of interpolation in obtaining KS
MNO	Order of interpolation in obtaining HS, HST, HK, CPK, HBRKN2, HBRNK02, MUK, and KGK
MPDOT	Effective mass injection rate at char surface

MQC	Order of interpolation in obtaining QC
MS	Molecular weight of carbon
MSDOT	Rate of char layer removal by first order oxidation at end of time step
MSDOTP	Rate of char layer removal by first order oxidation at start of time step
MSQPT	Order of interpolation in obtaining SQPT
MU	Viscosity of pyrolysis gas mixture, single subscript
MUK	Viscosity of gaseous species, single subscript
MUKT	Table of gaseous species viscosity versus temperature, double subscript
MUKTV	Dummy array defined in computing pyrolysis gas viscosity, single subscript
N	Dummy index
NCPP	Number of entries in CPPT table
NIT	Iteration count
NITA	Trigger, set to 1 after first iteration following $\dot{m}_g = 1.0 \times 10^{-3} \text{ kg/m}^2\text{-sec}$
NITC	Trigger, set to 1 after first iteration
NITG	Trigger, set to 1 if surface temperature changes more than .2% with respect to previous times
NITP	Trigger, set to 1 when $\dot{m}_g = 1.0 \times 10^{-3} \text{ kg/m}^2\text{-sec}$
NITS	Trigger used in computing CPK and HK
NKP	Number of entries in KPT
NKS	Number of entries in KST
NNO	Number of entries in HSTT, HKT, CPKT, MUKT, and KUPT
NQC	Number of entries in QCTAB

NRCT	Number of homogeneous chemical reactions treated
NRHOK	Trigger used in solving species continuity equation, single subscript
NSQPT	Number of entries in SQPT
NSTEP	Dummy index
P	Pyrolysis gas pressure at end of time step, single subscript
PA	"PA" coefficient in finite difference equation for pyrolysis gas pressure evaluated at the pyrolysis zone
PAB3 } PAB4 }	Coefficients in finite difference equation for pyrolysis gas pressure evaluated at mid-point of time step, single subscript
PAL1 } PAL2 } PAL3 } PAL4 }	Coefficients in linearized differential for pyrolysis gas pressure evaluated at end of time step, single subscript
PAMGDOT	Product of chemical species density and velocity at start of time step, double subscript
PAP1 } PAP2 } PAP3 } PAP4 }	Value of PAL1, etc. evaluated at the start of the time step, single subscript
PART	Parameter defined by $ TS(1)-TSP(1) $
PB	"PB" coefficient in finite difference equation for pyrolysis gas pressure evaluated at the pyrolysis zone
PD	"PD" coefficient in finite difference equation for pyrolysis gas pressure evaluated at the pyrolysis zone
PHBRKN2	Enthalpy of $N_2$ at char surface temperature evaluated at start of time step
PHBRK02	Enthalpy of $O_2$ at char surface temperature evaluated at start of time step
PHI	Parameter defined in computing viscosity of pyrolysis gas, double subscript

PM	Permeability of char layer at end of time step, single subscript
PMU	Pyrolysis gas viscosity at pyrolysis zone, evaluated at start of time step
PMV	Data input for permeability of char layer
PP	Pyrolysis gas pressure at start of time step, single subscript
PPM	Permeability of char layer at pyrolysis zone, evaluated at start of time step
PR	Prandtl number of pyrolysis gas
PRHO	Pyrolysis gas density at start of time step, single subscript
PRINTFQ	Time interval at which output is printed
PROM	Sum of mole density of all chemical species, single subscript
PROPC	Proportionality constant appearing in equation for HA
PSI	Parameter defined in computing conductivity of pyrolysis gas, double subscript
PT	Pyrolysis gas temperature at last table look up of data, single subscript
PTIME	Print time
PTS	Solid temperature at last table-look-up data, single subscript
PW	Dimensionless pressure at surface of char layer
PWP	Dimensional pressure at surface of char layer
PX )	"PX", etc. coefficients in finite difference equation for pyrolysis gas pressure evaluated the pyrolysis zone
PY )	
PZ )	
Q	Net heat transfer at char surface by conduction at end of time step

QC	Heat transfer to cold, non-ablating body
QCOND	Rate of energy transfer by conduction at char layer surface
QCT	Aerodynamic heat transfer to hot, ablating body
QCTAB	Table of QC versus time, single subscript
QFAC	Parameter define in computation of aerodynamic heat transfer
QNET	Heat transfer to back surface of insulation layer at end of time step
QPNET	Heat transfer to back surface of insulation layer at start of time step
QPT	Net heat transfer at char surface by conduction at start of time step
QRAT	Ratio of set heat transfer at surface by conduction to cold wall, non-ablating heat transfer
QRS	Radiant heat transfer at surface
RAD	Vehicle nose radius
RHO	Pyrolysis gas density at end of time step, single subscript
RHOK	Density of chemical species at end of time step, double subscript
RHOKP	Density of chemical species at start of time step, double subscript
RHOP	Density of uncharred layer at end of time step, single subscript
RHOPP	Density of insulation layer, single subscript
RHOPPV	Data input for insulation density
RHOSO	Density of char layer at front surface
RHOST	Theoretical density of char layer
RHR	Rate of function of chemical species by heterogeneous chemical reactions, double subscript



RHS	Rate of formation of solid by heterogeneous chemical reactions, single subscript
RJN	Rate of reaction of chemical reaction, single subscript
RM	Total mass rate of production, single subscript
RMP	Parameter defined by $\pi_1 (\rho_1/M_1)^{v''}$ , single subscript
RMR	Parameter defined by $\pi_1 (\rho_1/M_1)^{v'}$ , single subscript
ROCPM	Parameter defined by $\sum_i \rho_i C_{p_i}/M_i$ , single subscript
ROHM	Parameter defined by $\sum_i \rho_i H_i/M_i$ , single subscript
ROM	Total mole density of pyrolysis gas, single subscript
RS	Mole rate of production of solid carbon at end of time step, single subscript
RT	Mole rate of production of chemical species, double subscript
RU	Universal gas constant
S	Trigger for surface removal mechanism
SGMA	Stephan-Boltzmann constant
SP	Trigger for selecting mode of calculation of pyrolysis rate of uncharred layer
SPECIES	Identification of gaseous species, single subscript
SQPT	Table of $(PW)^{1/2}$ versus time, single subscript
T	Pyrolysis gas temperature at end of time step, single subscript
TCPP	Temperature table for CPPT, single subscript
TEMP	Temperature table for HSTT, HKT, CPKT, MUKT, and KUPT, single subscript
TF	Pyrolysis gas temperature in double precision, single subscript

TFS	Solid temperature in double precision, single subscript
TIBAR	Maximum temperature at pyrolysis zone
TIME	Time from start of program
TIMET	Time table for QCTAB, single subscript
TKP	Temperature table for KPT, single subscript
TKS	Temperature table for KST, single subscript
TMPRES	Time table for SQPT, single subscript
TP	Pyrolysis gas temperature at start of time step, single subscript
TRAB	Trigger for selecting blocking approximation
TREF	Transpiration effectiveness
TS	Solid temperature at end of time step, single subscript
TSAVE	Parameter used in calculating DHK
TSP	Solid temperature at start of time step, single subscript
T1BAR	Sublimation temperature of char layer
V	Average velocity of gas in char layer, single subscript
VC	Velocity of moving coordinate, single subscript
W	Parameter defined in algorithm for solving finite difference equations for pyrolysis gas pressure
WS	Parameter defined in algorithm for solving finite difference equations for solid temperature
X	Dimensionless char layer coordinate
XIS	Coefficient in solid temperature finite difference equation at the pyrolysis zone and the uncharred layer insulation layer interface
XP	Dimensionless coordinate in uncharred layer

XSCNST	Coefficient in solid temperature finite difference equation evaluated at the back surface of the insulation layer
YETA	Time derivative of char layer porosity, single subscript
YIS	Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer-insulation layer interface
YP	Time derivative of pyrolysis gas pressure, single subscript
YRHO	Time derivative of pyrolysis gas density, single subscript
YRHOK	Time derivative of gaseous chemical species density, double subscript
YSCNST	Coefficient in solid temperature finite difference equation evaluated at the back surface of the insulation layer
YT	Time derivative of pyrolysis gas temperature, single subscript
YTS	Time derivative of solid temperature, single subscript
ZIS	Coefficient in solid temperature finite difference equation evaluated at the pyrolysis zone and the uncharred layer insulation layer interface
ZP	Pyrolysis gas pressure in double precision, single subscript
ZSCNST	Coefficient in solid temperature finite difference equation evaluated at the back surface of the insulation layer

## VITA

The author was born [REDACTED] in [REDACTED]. After graduating from Lafayette High School in Mayo, Florida in 1955, he served three years on active duty with the U. S. Army before enrolling in the University of Florida. In 1962 he received the Bachelor of Mechanical Engineering Degree with Honors from the University of Florida and has been employed by the National Aeronautics and Space Administration at the Langley Research Center since that time. He has earned the Master of Aerospace Engineering Degree from the University of Virginia since being employed by NASA.

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